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ABSTRACT BOOK

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Preface:

CUI is not only providing quality education, but also producing the valued research publications. Due to this research work, the CIIT got its better ranking in Pakistan and Higher Education Commission declared CIIT at top ranking among Pakistani Universities. The credit goes to the researchers of CUI, who, as usual, produced lots of papers in the year 2020. For this accomplishment, the contribution of researchers of CUI Lahore is also extraordinary. They produced 276 journal papers during the year 2020. The compilation in your hands consists of the papers which published during the year 2020 and at CUI platform. We only included journal papers for this anthology. The purpose of this compilation is to record the research work of our faculty members and also to facilitate the users to get all the research papers of all departments in one binding. Apart from the record, I am also sure that this compilation will provide the guidelines to new researchers of CIIT and to the researchers of other institutes, as well. I am very much thankful to worthy Director CIIT-Lahore Dr. Asad Hussain and Dr. Muhammad Asif, Convener Library Affairs Committee, they not only provided the guidelines, but also encourage us to prepare this compilation in appropriate form. I am also very much thankful to ORIC, which provided the data to compile this report. Without this help, it was very difficult to prepare this collection of research articles.

With Regards

DR. MUHAMMAD TARIQ

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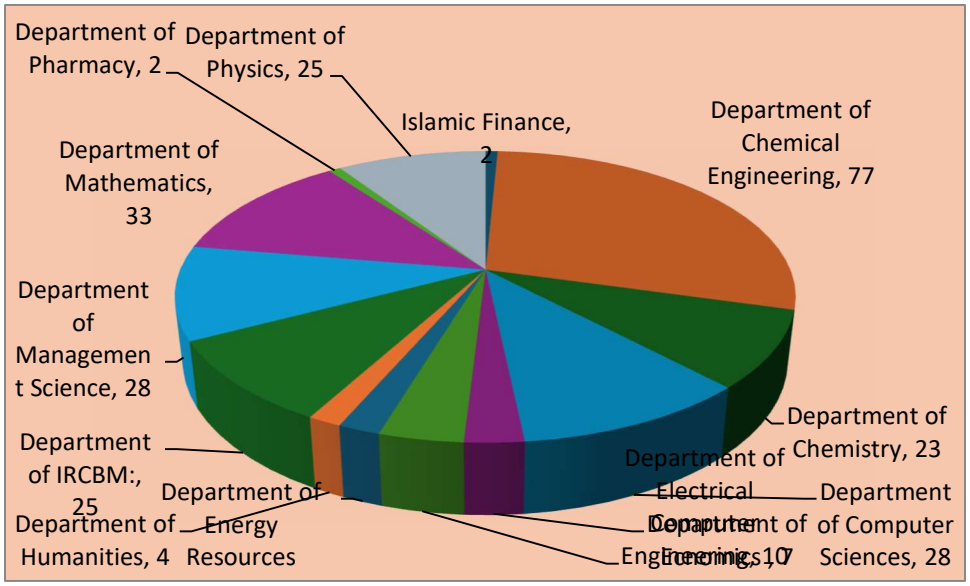

CENTER OF ISLAMIC FINANCE

1. Ali, I., Akhter, W., & Chaudhry, N. (2023). Do Islamic Holy days affect stock returns? Empirical evidence from Asian and African markets. *Journal of Islamic Marketing*, *14*(1), 273-288.

ABSTRACT:

Purpose

The Islamic Holy days are among the most celebrated spiritual traditions in the world and are observed by more than 1.5 billion Muslims. This study aims to investigate the effect of these events on the regular returns of stock exchanges in selected Muslim countries.

Design/methodology/approach

This study examines data from eight Asian and African stock exchanges from 2001 to 2019. Isolating the effect of Gregorian calendar anomalies, it aims to evaluate the effect of Islamic Holy days on stock returns by running a pooled random effect panel regression on all the stock exchanges examined.

Findings

The results reveal the positive impact of Eid-ul-Fitr on Asian markets, the negative impact of Eid Milad-un-Nabi on the African stock market's returns and the positive effect of the Holy month of Ramadan on both markets. Some Gregorian calendar anomalies also were found in these markets.

Practical implications

The research has significant implications for marketing professionals to recognize business opportunities and investors to efficiently manage their stock portfolio during Islamic events of Eid-ul-Fitr, Eid Milad-un-Nabi and Ramadan in relevant Muslim countries.

Originality/value

Given the research gap between Gregorian and Islamic calendar anomalies, this paper contributes by combining the effect of Islamic Holy days on the returns of selected Muslim-dominated financial markets

Web URL: https://www.emerald.com/insight/content/doi/10.1108/JIMA-09-2020-0285/full/html

2. Zaman, Q. U., Akhter, W., Abdul-Majid, M., Hassan, S. I. U., & Anwar, M. F. (2023). Does bank affiliation affect firm capital structure? Evidence from a financial crisis. Journal of Economic and Administrative Sciences, 39(1), 150-174.

ABSTRACT:

Purpose

This study aims to assess the determinants of corporate debt with a particular focus on bank-affiliated and non-bank-affiliated firms during the global financial crisis.

Design/methodology/approach

The authors analyse the data of 395 listed manufacturing firms from Pakistan with 2,370 firm-year observations. The sample is divided into subsamples, namely bank-affiliated, non-bank-affiliated and stand-alone firms. Fixed and panel effect regression models are applied to determine the during, pre-crisis and post-crisis effects on corporate capital structure.

Findings

The robust results of the study reveal that non-bank-affiliated firms have different leverage determinant behaviours with a greater reliance on size, tangibility and profitability. However, bank-affiliated firms seemed to show greater immunity from a crisis compared to other firms. Simultaneously, the stand-alone firms remained at a disadvantage subject to internal financial ties of group-affiliated firms and form a base of market imperfection.

Practical implications

This study's findings imply that financial managers should contain better ties with financial institutions to enhance financial immunity in worse time of financial crisis or COVID-19 global calamity. On the regulation front, these findings call for critical policy regulations to govern the internal ties with financial institutions to create a level playing field for the corporate sector.

Originality/value

To the best of the authors' knowledge, this study is the first to investigate determinants of corporate debt with a particular focus on bank-affiliated and non-bank-affiliated firms. This work is also novel to explore corporate debt of bank-affiliated and non-bank-affiliated firms during the financial crisis.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/JEAS-11-2020-0193/full/html

3. Usman, M., Akhter, W., & Haque, A. (2023). Spillover effects of crash and jump events: evidence from Chinese market. *China Finance Review International*, *13*(4), 599-620.

ABSTRACT:

Purpose

This paper aims to investigate the spillover effects of jump and crash events among Chinese nonfinancial firms.

Design/methodology/approach

This sample consists of more than 1.5 million weekly observations of over 3,000 Chinese listed firms over the period 1991–2015. The authors utilize univariate tests to compare the post-event performance of matched peer and non-peer control firms and cross-sectional regressions of their abnormal returns/cumulative abnormal returns (ARs/CARs) and returns on assets (ROAs).

Findings

The authors find that extreme risk-adjusted abnormal stock returns (stock price crashes and jumps) generate statistically significant ARs/CARs in the same directions in industry, size, leverage, and geographical location matched peer firms in Chinese stock market. Further tests reveal that peer firms' response to the crash event is pronounced more in the group of firms about which the information asymmetry is high between investors and firms.

Research limitations/implications

Portfolio investors can adjust their portfolios accordingly by selling stocks of the matching rival firms during a crash period. Policymakers may develop policies so as to protect the interests of small investors in the events of crashes in the markets. They can reduce the information asymmetry between the firms and the investors by making information about the firms more transparent, so as to reduce the contagion in case of crash event.

Practical implications

This study has important implications for portfolio investment managers and policymakers.

Originality/value

To the best of authors' knowledge, this is the first study that combines the jump and crash events and attempts to assess their spillover effects on other firms in Chinese stock market.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/CFRI-07-2022-0126/full/html

4. Usman, M., Li, C., Chaudhry, N., & Akhter, W. (2023). Does religion impact corporate innovation in developing countries?. Journal of Islamic Accounting and Business Research, 14(6), 887-910.

ABSTRACT:

Purpose

This study aims to examine how religion affects corporate innovation in developing countries.

Design/methodology/approach

Firm- and country-level indicators are used to evaluate the relationship. The study's final sample consists of manufacturing firms from 41 developing countries across different world regions from 2014 to 2018.

Findings

This paper finds that firms operating in more religiously diverse countries with lower religious restrictions are likely to be more innovative. Furthermore, secularization stimulates corporate innovation in contrast to traditional religious societies. Interestingly, results also indicate that

religion hinders corporate innovation by restraining its followers' involvement in innovative activities under risk, which downgrades corporate innovation culture.
Research limitations/implications
This study used data from nonfinancial firms from developing countries; therefore, the study's findings could be generalized to other developing economies with caution, as economies operating at different stages of development can have different outcomes from the proposed relationship. The study findings are important for innovative firms, as they can take advantage by segmenting the population based on religious and atheist groups. Results also have some implications for developing countries to foster firm-level innovation through constructing effective policies and ensuring the development of diverse and free religious societies because such societal traits increase corporate innovation and are fruitful for national competitiveness and growth.
Originality/value
This study contributes to institutional economics and corporate innovation by exploring the link between religion and economic development through the innovation channel and analyzing the latest cross-country evidence. It is a pioneering work in empirical comparison of influence on innovations of different religions.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/JIABR-10-2022-0258/full/html

5. Usman, M., Li, C., Chaudhry, N., & Akhter, W. (2023). Does religion impact corporate innovation in developing countries?. *Journal of Islamic Accounting and Business Research*, *14*(6), 887-910.

ABSTRACT:

Purpose
This study aims to examine how religion affects corporate innovation in developing countries.
Design/methodology/approach
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relationship. The study findings are important for innovative firms, as they can take advantage by segmenting the population based on religious and atheist groups. Results also have some implications for developing countries to foster firm-level innovation through constructing effective policies and ensuring the development of diverse and free religious societies because such societal traits increase corporate innovation and are fruitful for national competitiveness and growth.

Originality/value

This study contributes to institutional economics and corporate innovation by exploring the link between religion and economic development through the innovation channel and analyzing the latest cross-country evidence. It is a pioneering work in empirical comparison of influence on innovations of different religions.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/JIABR-10-2022-0258/full/html

6. Atif, R. M., Ahmed, F., Naveed, Z., & Abbas, G. (2024). CAUSAL NEXUS BETWEEN IMPORTS AND ECONOMIC GROWTH IN PAKISTAN: EVIDENCE FROM TODA-YAMAMOTO CAUSALITY TEST. *International Journal of Contemporary Issues in Social Sciences. ISSN (E) 2959-2461 (P) 2959-3808*, *3*(1), 336-345.

ABSTRACT:

Growth in the level of imports shows a strong domestic demand and a rising economy, particularlywhen these imports are productive and useful assets. However, there is a dearth of research carried on the relationship between GDP growth and imports. This research used Toda-Yamamoto Causality to investigate how imports affect Pakistan's economic growth. The years 1972 through 2020 are covered by yearly time series data. The study's findings suggest a long-run equilibrium relationship with bidirectional causality between imports and real GDP growth in Pakistan. Thus, it is proven that increasing imports will spur GDP growth in the long run. Whereas, in the short run true economic growth may result in an increase in the country's import demand. For a growing country like Pakistan, these two findings are very significant given the current scenario.

Web URL: http://ijciss.org/index.php/ijciss/article/view/316

DEPARTMENT OF CHEMICAL ENGINEERING

1. Iftekhar, H., Umair, M., Hamdani, S. T. A., Imran, S. M., Nazir, M. S., & Ali, Z. (2023). Effect of Hybrid Weave Patterns on the Mechanical Performance of Woven Fabrics. Journal of Natural Fibers, 20(1), 2145411.

ABSTRACT:
Improvement in mechanical properties of the natural fiber reinforcement for potential use in the composite for mechanical performance is a key focus of researchers in recent years. However, few studies are available in the literature on the mechanical performance of hybrid-woven fabrics. In this article, the effect of the weave structure of reinforcing fabric on mechanical performance has been investigated. Jute-based woven fabrics having four different weave structures (matt, sateen, and hybrid-weave A/B) were developed in the in-house lab using a shuttle dobby weaving machine. The tensile test and puncture tests were performed to evaluate the mechanical performance by varying the weave architecture. The sateen weave exhibited maximum penetration load during a puncture test. The results demonstrated a significant improvement in the tensile strength by using a hybrid weave in the warp direction. However, sateen woven fabric demonstrated enhancement in the tensile attributes in the weft-wise direction. Similarly, a hybrid weave consisting of a combination of sateen and matt weave exhibited a maximum stiffness value. To check the statistical significance of the results, ANOVA analysis was performed. The findings of ANOVA suggest that the results are statistically significant. This research will open a new avenue in the field of reinforcement composite material.

Web URL: https://www.tandfonline.com/doi/full/10.1080/15440478.2022.2145411

2. Iqbal, M. S., Nazir, M. S., Ali, Z., Iftikhar, R., Hussain, M., & Imran, S. M. (2023). Reduced graphene oxide coated poly-methyl methacrylate beads based thermoplastic polyurethane nanocomposites for gas sensing applications. *Polymer-Plastics Technology and Materials*, *62*(6), 790-799.

ABSTRACT:
We have fabricated, reduced graphene oxide (rGO) coated poly methyl methacrylate (PMMA) based thermoplastic polyurethane (TPU) nanocomposites for NO_2 gas sensing. The rGO-coated PMMA beads and MWCNTs were incorporated into the TPU matrix in different concentrations by melt mixing. The characterization was done to confirm the preparation of the nanocomposites. The rGO-coated PMMA-TPU nanocomposites exhibit excellent electrical conductivities and efficient NO_2 gas sensing. The developed sensor can sense NO_2 at room

temperature with the highest response time of 19 s and an average response time of 23.67 s. The sensor is recovered within 31.4 s and has a limit of detection of 9.51 ppm.

Web URL: https://www.tandfonline.com/doi/full/10.1080/25740881.2022.2150864

3. Younas, M., Shafique, S., Faisal, A., Hafeez, A., Javed, F., Mustafa, M., & Rehman, F. (2023). Hydrogen production through water vapors using optimized corona-DBD hybrid plasma micro-reactor. *Fuel*, *331*, 125838.

ABSTRACT:
Hydrogen as secondary energy carrier is one of the promising routes to meet renewable and sustainable energy demand. Hydrogen production using water plasmolysis, so far, has been considered as energy intensive. However, recent developments in the field of microplasmas has reduced energy requirement of water plasmolysis on par with electrolysis. However, there's still room for improvement as water vapors dissociation efficiencies are less than thermodynamic and kinetic limits. One of the ways to do that is to split microchannel in plasma into sub-micron channels by packing beads inside the reactor. The current study investigates the plasmolysis of water vapours (steam) and argon gas with (1) empty channel plasma reactor and (2) glass beads packed plasma reactor. A custom-made Corona-DBD hybrid microplasma reactor has been designed and employed for water steam plasmolysis. This study aims to investigate the feasibility of water vapors dissociating into hydrogen at a relatively small interelectrode gap at atmospheric pressure. The minimum breakdown voltage has been found to be 3.7 kV_{pk-pk} at 5 mA current. The maximum hydrogen production rate was observed 23.9 g/kWh at optimized conditions for the glass beads packed plasma reactor. So, in current study glass beads packed plasma microreactor yielded 23.9g of H_2/kWh which is significantly higher than any previously published study

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122026643

4. Bhavani, P., Kumar, D. P., Yoo, J. S., Hussain, M., Weon, S., Kim, W., & Park, Y. K. (2023). Dual-Atomic-Site-Integrated Photocatalysts for Green Energy Synthesis. *Chemical Engineering Journal*, 143429.

ABSTRACT:
Dispersing active metals into theoretical atomic level has emerged as a cost-effective means for constructing catalysts, which are considered single-atom catalysts (SACs). SACs are integrated with various photocatalysts to serve as efficient platforms for solar energy conversion. Though SACs exhibit superior catalytic activity and selectivity owing to their maximum atomic utilization and high versatility of surrounding atomic configurations, the nature of SACs containing only one type of active site limits various chain reactions, inhibiting catalytic performance. To overcome these limitations, dual atom catalysts (DACs) have emerged as a new inventive material for boosting photocatalytic reactions. Thus, this review discusses the limitations of SACs and relative advantages of DACs, synthesis of dual atom sites on various substrates, identification of dual atomic sites through characterizations, and applications of

DACs in various photocatalytic energy harvesting such as H_2 production, CO_2 reduction, and N_2 reduction. Finally, perspectives and future directions for increasing the photocatalytic performance of DACs-integrated photocatalysts are proposed.

Web URL: https://www.sciencedirect.com/science/article/pii/S1385894723021605

5. Ahmad, N., Ahmad, N., Ahmed, U., Jameel, A. G. A., Hussain, M., & Arif, M. M. (2023). Production of fuel oil from elastomer rubber waste via methanothermal liquefaction. *Fuel*, *338*, 127330.

ABSTRACT:

The amount of rubber waste is increasing globally due to its use in various industries. This waste rubber do not degrade and it remains in the environment for a long period of time. Polymer recycling industry is in good position to address the issue of rubber waste by converting it into fuel. Fuel oil was produced through the thermal liquefaction of natural rubber polymer, using methanol as a solvent. A kettle batch type reactor was used for the conduction methanothermal liquefaction of natural rubber. Various set of experiments were performed for the synthesis of fuel oil by manipulating the process parameters such as temperature (from 250 °C to 375 °C), methanol to natural rubber ratio (from 0.5/1 to 4/1), and reaction times (from 0.25 h to 1.25 h). The results showed that the highest yield of 79 % of fuel oil was obtained from the methanolysis of natural rubber which was 21.36 % higher than the oil synthesized via pyrolysis of tire rubber. The results of Gas chromatography–mass spectrometry (GC–MS) indicated the presence of limonene about 42 % in oil derived from natural rubber, while the bio-oil obtained from the pyrolysis of tire rubber and natural rubber yields approximately 25 % and 32 % of limonene respectively. Also, the presence of alkyl derived groups and methylene groups were recognized as the supreme leading functional groups present in fuel oil. The elemental analysis showed that in comparison to natural rubber, the high amount of sulfur was present in tire rubber based oil makes it corrosive and toxic.

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122041540

6. Jamil, F., Shafiq, I., Sarwer, A., Ahmad, M., Akhter, P., Inayat, A., ... & Hussain, M. (2024). A critical review on the effective utilization of geothermal energy. *Energy & Environment*, *35*(1), 438-457.

ABSTRACT:

Rapid growth in the global population and associated elevated reliance on modern technology has resulted in increased demand for energy consumption. This has resulted in an increased focus on the development and generation of advanced sustainable energy systems. The swift implementation of sustainable renewable energy resource utilization and improvement in their efficiency by the modification of current technologies are the possible solutions that gave rise to the emergence of geothermal technology as a potential alternative. Geothermal technology is a non-carbon renewable energy resource that could be utilized efficiently to fulfil the energy demands while mitigating the climate change threat. According to the surveyed literature, the global geothermal energy power plant installation capacity has reached 14.3 GWe to successfully implement this sustainable alternative. In order to have a successful and uninterrupted way forward, it is essential to evaluate the constraints both in terms of technicality and economic

feasibility to establish an approved framework. Moreover, the governance and monitoring regarding the social and environmental impact alongside the legal challenges should also be addressed. The significant barriers include increased capital cost, site selection, superiority of resources at diverse levels of rock bottoms, and obstruction from nearby residents that need to be addressed appropriately. As a result, policymakers will continue to seek measure that have least negative impact on environment.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/0958305X231153969

7. Jamil, F., Saleem, M., Qamar, O. A., Khurram, M. S., Ala'a, H., Inayat, A., ... & Park, Y. K. (2022). State-of-the-art catalysts for clean fuel (methyl esters) production-A comprehensive review. *Journal of Physics: Energy*.

ABSTRACT:

There has been growing and recent interest in using non-edible feedstocks, such as waste animal fats, as an alternative to vegetable oils in biodiesel production to address the food versus fuel debate. Waste animal fats are cost effective and yield good quality biodiesel. Therefore, waste animal fats are appealing and excellent feedstocks to produce biodiesel. Commercially, the biodiesel is obtained by transesterification reaction of triglycerides present in oil/fat with alcohol in the presence of homogeneous base catalysts. However, free fatty acids found in low-quality oil feedstocks are particularly sensitive to homogeneous base catalysts, necessitating extra acid pretreatment and neutralization procedures that not only raise the overall expense of producing biodiesel but also create environmental contamination. Optimistically, the use of solid catalysts can offer an environmentally friendly, cost-effective and practical route for the manufacture of biodiesel from inexpensive oil feedstocks, including waste animal fat. The present review article covers catalyzed transesterification/esterification using various catalysts with particular focus on the use of heterogeneous catalysts when using waste animal fat as feedstock for biodiesel production. In particular, the properties of biodiesel obtained from waste animal fats are also compared to the biodiesel properties of standard organizations, such as the European Committee for Standardization (ISO) and the American Society for Testing and Materials (ASTM). Moreover, this paper also offers future research directions that can direct researchers to fill in knowledge gaps impeding the creation of efficient heterogeneous catalysts for long-term biodiesel generation. To the best of our knowledge, the valorization of waste animal fats from slaughterhouses is not feasible and has some techno-economic concerns. However, this technology is more desirable considering the environmental point of view to address the pollution problems caused by these wastes.

Web URL: https://iopscience.iop.org/article/10.1088/2515-7655/aca5b3/meta

8. Hussain, S., Wadgama, M. H., Khan, A. L., Yasin, M., & Akhtar, F. H. (2023). Upcycling Poly (ethylene terephthalate) by Fabricating Membranes for Desalination. *ACS Sustainable Chemistry & Engineering*, *11*(2), 726-732.

ABSTRACT:

Waste plastic upcycling is attracting increasing attention as a green and sustainable route for membrane fabrication. However, the existing literature in this domain is limited only to few commercial applications. This work presents the performance of membranes synthesized from recycled poly(ethylene terephthalate) (PET) for water desalination. PET extracted from waste plastic bottles was used to produce asymmetric membranes via nonsolvent-induced phase separation. The membrane performance was optimized by fine-tuning the PET, cosolvent, and additive concentration and the coagulation bath temperature. Increasing the PET content in the casting solution led to a decline in permeance across all experiments. A higher % composition of the volatile cosolvent in the solution improved the membrane selectivity. The addition of poly(ethylene glycol) as a pore-forming agent enhanced the permeance, and a higher NaCl rejection was observed when the coagulation bath temperature was decreased from 25 to 0 °C. Subsequently, PET membranes were also used as a support to fabricate thin-film composite membranes via interfacial polymerization of trimesoyl chloride and piperazine. These membranes demonstrated a remarkable permeance of 73 ± 4 L m^{-2} h^{-1} bar^{-1} with a 33 ± 2% NaCl rejection. The findings of this study offer promising prospects for developing high-performance membranes using commercial plastic waste.

Web URL: https://pubs.acs.org/doi/full/10.1021/acssuschemeng.2c05964

***9.* Ahmad, M., Zafar, M., Bokhari, A., Akhtar, M. S., Alshgari, R. A., Karami, A. M., & Asif, S. (2023). Membrane reactor for production of biodiesel from nonedible seed oil of Trachyspermum ammi using heterogenous green nanocatalyst of manganese oxide. Chemosphere, 322, 138078.**

ABSTRACT:

Conventional homogeneous-based catalyzed transesterification for the production of biodiesel can be replaced with a membrane reactor that has an immobilized heterogeneous catalyst. Combining reaction with separation while utilizing membranes with a certain pore size might boost conversion process. this investigation to study the effectiveness of membrane reactor in combination with heterogeneous green nano catalysis of MnO_2. Techniques such as XRD, EDX, FTIR, SEM, and TGA were used to characterize the synthesized MnO_2 nano catalyst. The highest conversion of around 94% *Trachyspermum ammi* oil was obtained by MnO_2. The optimum process variables for maximum conversion were catalyst loading of 0.26 (wt.%), 8:1 M ratio, 90 °C reaction temperature, and time 120 min. The green nano catalyst of MnO_2 was reusable up to five cycles with minimum loss in conversion rate of about 75% in the fifth cycle. Nuclear magnetic resonance validated the synthesis of methyl esters. It was concluded that membrane reactor a promising technique to efficiently transesterify triglycerides into methyl esters and enable process intensification uses MnO_2 as a catalyst.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653523003454

10. Dilpazeer, F., Munir, M., Baloch, M. Y. J., Shafiq, I., Iqbal, J., Saeed, M., ... & Mahboob, I. (2023). A Comprehensive Review of the Latest Advancements in Controlling Arsenic Contaminants in Groundwater. Water, 15(3), 478.

ABSTRACT:
Water contaminated with arsenic is a worldwide problem. This review presents the arsenic contamination in groundwater, its sources, and possible health risk to humans. Groundwater pollution is the most common route of inorganic arsenic exposure in humans. Arsenic concentrations in different countries were analyzed and projected on a map. Because arsenic is widely spread throughout the Earth's crust, it is present in trace amounts in practically all waterways. Harmful levels of this toxin have been identified in drinking water in some regions. For drinking purposes, the majority of people use groundwater; excess arsenic levels in groundwater have been linked to a variety of negative health impacts on people. Arsenic exposure is the world's leading environmental cause of cancer. The main aim of this review is to summarize the effective technologies to remove arsenic from drinking water, such as ion exchange, coagulation/flocculation, and membrane technologies like ultra-filtration and electrodialysis, helping to deal with the adverse effects caused by arsenic exposure. All these technologies present different advantages and disadvantages. Electrocoagulation, adsorption, and phytoremediation are the most efficient and cost-effective technologies. The removal efficiencies of arsenic using these technologies and prospects were also included.

Web URL: https://www.mdpi.com/2073-4441/15/3/478

11. Bhavani, P., Kumar, D. P., Hussain, M., Chen, W. H., Lam, S. S., & Park, Y. K. (2023). Surface ligand functionalized Few-layered MoSe2 nanosheets decorated CdS nanorods for spectacular rate of H2 production. Fuel, 334, 126551.

ABSTRACT:
The properties of few-layered transition metal dichalcogenides (TMDs) are extremely interesting in the category of two-dimensional (2D) materials due to their feasibility of band gap engineering, high carrier mobility, and the ability to tune carrier concentration, which makes its utilization in wide range application. In the current study, we report the conversion of $MoSe_2$ multilayers into a few layers as well as tune its band gap and band potentials by surface organic ligand (benzylamine) functionalization. Further, this functionalized few-layered $MoSe_2$ has been deposited on CdS nanorods and tested for photocatalytic H_2 production through water splitting under solar similar light excitation. Consequently, the optimized BA-$MoSe_2$/CdS composites generated efficient hydrogen (54.9 $\mu mol \cdot h^{-1}\ g^{-1}$) production, which is 3 and 18 folds enhanced than the simple few-layered $MoSe_2$/CdS and CdS, respectively. The decoration of a few layered BA-$MoSe_2$ on CdS nanorods effectively alters the band potentials suitably for proton reduction, then, separated greater photo-induced chargers, thereby, improving electrons accommodation on the catalysts surface and transferring to the active sites. Particularly, these outcomes would give a potential prospect for prominent photocatalytic systems development owing to their spectacular photo-efficiency and economic feasibility.

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122033750

12. Ali, Z., Naz, A., Haq, N. U., Nazir, A., Munawar, A., Khan, A. L., ... & Iqbal, M. (2023). Fabrication of novel Zn (II)-imidazole based mixed matrix membranes for heavy metal removals from drinking water. Zeitschrift für Physikalische Chemie, (0).

ABSTRACT:
Heavy metals presence in the potable water is a terrible dilemma notably for emergent countries and could be carcinogenic. Currently, interfacial polymerization (IP) was applied for the production of thin film nanocomposite forward osmosis (TFN-FO) membrane using polyacrylonitrile support. For this purpose, Zn (II)-imidazole metal Organic framework (MOF) was employed as a nanofiller into polymeric membranes this modification was found useful for the removal of heavy metals. Different characterization techniques like scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDS), Fourier transform infra-red spectroscopy (FTIR) and X-ray diffraction (XRD) analyses were used for the assessment of morphology, elemental arrangement, functional groups and crystalline nature of the prepared FO membrane. It was observed that synthesized Zn-MOF based FO membrane displays high water flux by increasing the number of pores in the membrane. Additionally, this particular FO membrane was custom-made for lower reverse solute flux and concentration polarization. This ensures minimum withdrawal of salt from the draw solution (DS) to the feed solution (FS). So, the prepared Zn-MOF based FO membrane produce synergistic outcomes for the removal of metals and this strategy could possibly be used as novel way for removal of toxic pollutants.

Web URL: **https://www.degruyter.com/document/doi/10.1515/zpch-2023-0230/html**

13. Ullah, Z., Kainat, F., Manzoor, S., Liaquat, H., Waheed, A., Akhtar, S., ... & Razaq, A. (2023). Natural fibers and zinc hydroxystannate 3D microspheres based composite paper sheets for modern bendable energy storage application. Journal of Applied Polymer Science, 140(1), e53275.

ABSTRACT:
For modern high-tech flexible energy storage devices, it becomes important to synthesize micro-/nanostructures as per the required shape and morphology with superior physical and electro-active characteristics. This work shares the fabrication and characterization of $ZnSn(OH)_6$ (Zinc hydroxystannate [ZHS]) prepared by facile microwave-assisted technique and furthermore converted into flexible sheets by employing lignocelluloses (LC) known as natural fibers, collected from Carica papaya leaf petiole as a substrate to provide the flexible matrix. X-ray diffraction measurements confirm the successful crystalline structure of ZHS. Scanning electron microscopy and transmission electron microscopy showed the solid spherical structure of ZHS microspheres. Fourier transform infrared spectrometry and Raman spectroscopy confirmed the composite formation of ZHS and LC-based composite sheets (ZHS/LC sheets). Electrochemical measurements that is, cyclic voltammetry (CV), Galvanostatic charge/discharge, and electrochemical impedance (EIS) spectroscopy revealed the electroactive behavior of ZHS/LC paper sheets as working electrode for energy storage applications. CV measurements revealed the specific capacitance of 100 F/g and EIS measurements confirmed the decrease in the resistance of LC fiber after the growth of ZHS microspheres. Presented flexible ZHS based paper

sheets will be highly feasible for the modern bendable/flexible/disposable energy storage applications.

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/app.53275

***14*. Saleem, A., Farooq, U., Riaz, A., Ahmed, F., Hussain, A., & Lee, M. (2023). Understanding the impact of reactive holdup on process intensification in the design of reactive distillation column. Chemical Engineering and Processing-Process Intensification, 109440.**

ABSTRACT:
The commercial viability of reactive distillation as a front-runner industrial process intensification technique is limited by slow reactions. It is because the diameter established by the vapor-loading method restricts large holdup volumes (or catalyst amount) to accomplish the essential conversion. However, placing a large amount of catalyst on column trays necessitates either a high tray weir height (limited to excessive column pressure drop) or a large column diameter. This study aims to investigate an alternative design approach by increasing the column diameter beyond that required for vapor loading to retain a large holdup volume. Several combinations of tray weir heights and column diameters were studied and demonstrated through case studies for three industrial processes, and their optimal designs have been reported. High catalyst holdup volume enhanced energy efficiency and overcame hydraulic limitations despite requiring large diameter vessels. These design configurations with optimized catalyst holdup also resulted in improved process economics. Fabricating a wide column diameter is a good conservative engineering procedure considering safety aspects and better design control.

Web URL: https://www.sciencedirect.com/science/article/pii/S0255270123001770

***15*. Khalid, M. T., Anjum, T., Khan, A. L., Rehman, F., Aslam, M., Gilani, M. A., ... & Yasin, M. (2023). Task-specific polymeric membranes to achieve high gas-liquid mass transfer. Chemosphere, 313, 137603.**

ABSTRACT:
In the current study, Polyimide (P84)-based polymeric membranes were fabricated and used as spargers in the bubble column reactor (BCR) to get a high gas-liquid mass transfer (GL-MT) rate of oxygen in water. Different polymeric membranes were fabricated by incorporating polyvinyl pyrrolidone (PVP) as a porogen and a Zeolitic Imidazolate Framework (ZIF-8) to induce high porosity and hydrophobicity in the membranes. The GL-MT efficiency of membranes was evaluated by measuring the overall volumetric mass transfer coefficient (k_La) of oxygen in air. The k_La of O_2 (in air) was measured by supplying the gas through a fixed membrane surface area of 11.94 cm^2 at a fixed gas flow rate of 3L/min under atmospheric pressure. The results revealed that adding porogen and ZIF-8 increased the porosity of the membranes compared to the pure polymeric membranes. In comparison, the ZIF-8 (3 wt%) based membrane showed the highest porosity (80%), hydrophobicity (95° contact angle) and k_La of oxygen in air (241.2 h^{-1}) with 78% saturation in only 60 s. ZIF-8 based membranes showed the potential to increase the amount

of dissolved oxygen in BCR by reducing the bubble size, increasing the number of bubbles, and improving the hydrophobicity. The study showed that ZIF-8 based membrane diffusers are expected to produce high GL-MT in microbial syngas fermentation. To the best of our knowledge, this is the first study on the fabrication and application of polymeric membranes for GL-MT applications. Further research should be conducted under real fermentation conditions to assess the practicality of the system to support substrate utilization, microbial growth, and product formation.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0045653522040966**

16. Klemeš, J. J., Foley, A., You, F., Aviso, K., Su, R., & Bokhari, A. (2023). Sustainable energy integration within the circular economy. Renewable and Sustainable Energy Reviews, 177, 113143.

ABSTRACT:
This Virtual Special Issue (VSI) presents a selection of the presentation at the 24th Conference of Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES'21), which was held as a hybrid (face2face + online) conference in Brno, Czech Republic, on the 31st October to the November 3, 2021. The main features were related to the scope of Renewable and Sustainable Energy. Topics covered in this VSI also include climate and emission neutrality of energy systems, sustainable energy systems optimisation, energy recovery and integration. Topics covered in this VSI also cover circular economy, which has been identified as a viable strategy towards achieving sustainable development. It aims to decouple economic growth from resource use and waste generation. However, most technologies that promote circularity necessitate increased energy use to enhance material recovery and recycling. To ensure that the advances made in creating a more circular economy are not in conflict with mitigating climate change and achieving close to net zero emissions by 2050, a portfolio of technologies and strategies that reduce the carbon emissions intensity of the energy sector should be implemented. Climate and emission-neutral energy systems that utilise renewable energy, such as solar and geothermal power, decarbonise the energy sector's emissions. Developing more sustainable and renewable energy devices such as photovoltaic/thermal collectors, phase change materials, and solar devices, together with establishing infrastructure that supports these technologies, such as 6G wireless networks, would improve efficiency during energy generation, transmission, and use. The design and implementation of energy recovery and integration networks would reduce operational energy requirements in process industries. Finally, to maximise the benefits derived from these strategies, optimisation models which consider temporal and geographical constraints should be developed to determine their proper deployment. Sustainable development could be achieved by successfully integrating sustainable energy within a circular economy.

Web URL: https://www.sciencedirect.com/science/article/pii/S1364032122010243

17. Li, X., Liu, G., Zheng, H., Sun, K., Wan, L., Cao, J., ... & Bokhari, A. (2022). Recent advances on heteroatom-doped porous carbon—based electrocatalysts for oxygen reduction reaction. Energies, 16(1), 128.

ABSTRACT:
Polymer electrolyte membrane fuel cells are considered one of the alternatives to fossil energy sources. The slow kinetics of the oxygen reduction reaction (ORR) at the cathode and the high price of Pt-based catalysts remain one of the key challenges for the commercial viability of proton exchange membrane fuel cells. However, their high cost and susceptibility to poisoning severely limit their use for large-scale commercial applications in fuel cells. Heteroatom-doped porous carbon has attracted extensive attention from scientists due to its advantages such as high specific surface area and the properties conferred by heteroatom doping. On the one hand, we discuss a variety of current methods for the preparation of heteroatom-doped porous carbons, including the template method and the activation method. On the other hand, we discuss the application of heteroatom-doped porous carbon in Pt catalysts, transition metal catalysts and metal-free catalysts. Finally, we also present the pre-existing and challenges of heteroatoms in ORR catalysis, which will drive the development of ORR catalysts.

Web URL: https://www.mdpi.com/1996-1073/16/1/128

18. Shahid, M. K., Mainali, B., Rout, P. R., Lim, J. W., Aslam, M., Al-Rawajfeh, A. E., & Choi, Y. (2023). A Review of Membrane-Based Desalination Systems Powered by Renewable Energy Sources. Water, 15(3), 534.

ABSTRACT:
The rising demand for clean water and the environmental challenges associated with fossil fuels have encouraged the application of renewable and greener energy systems in desalination. Moreover, the small footprint and high productivity favored the membrane-based process in the water industry. In the past few decades, noticeable work has been performed on the development and applicability of membrane-based desalination processes powered by renewable energy sources such as solar, wind, tidal, and geothermal. Several integrated membrane desalination processes for producing clean water with sustainable and clean energy are introduced. This review details the source and performance efficiencies of existing renewable energy technologies and their application in membrane-based desalination processes, with a special focus on current advancements and challenges. This study reviews the interconnections between water, energy, and the environment and explores future energy-efficient desalination options for energy savings and environmental protection.

Web URL: https://www.mdpi.com/2073-4441/15/3/534

19. Rehman, F., Parveen, N., Iqbal, J., Sayed, M., Shah, N. S., Ansar, S., ... & Boczkaj, G. (2023). Potential degradation of norfloxacin using UV-C/Fe2+/peroxides-based oxidative pathways. Journal of Photochemistry and Photobiology A: Chemistry, 435, 114305.

ABSTRACT:
The removal of norfloxacin (NOR), a widely used pharmaceutical and emerging water pollutant, was studied using UV-C and Fe^{2+} catalyzed peroxides-based oxidative processes (e.g., UV-C/Fe^{2+}/H_2O_2, UV-C/Fe^{2+}/$S_2O_8^{2-}$ and UV-C/Fe^{2+}/HSO_5^-) and compared with UV-C and UV-C/Fe^{2+}. The UV-C and UV-C/Fe^{2+} degraded NOR to 38 and 55 %. However, use of peroxides, i.e., H_2O_2, $S_2O_8^{2-}$, HSO_5^- with UV-C and UV-C/Fe^{2+} promoted NOR %degradation to 75, 83, and 90 % using $[peroxides]_0 = 50$ mg/L, $[Fe^{2+}]_0 = 1$ mg/L, and $[NOR]_0 = 10$ mg/L, respectively. The significant impact of peroxides on NOR degradation was due to their decomposition into $^{\bullet}OH$ and $SO_4^{\bullet-}$ which showed high activity towards NOR degradation. The $^{\bullet}OH$ and $SO_4^{\bullet-}$ formation from peroxides decomposition and their contribution in NOR degradation was verified by different scavenger studies. Among the UV-C/Fe^{2+}/peroxides processes, UV-C/Fe^{2+}/HSO_5^- showed better performance. The changing concentrations of peroxides, Fe^{2+}, and NOR affected degradation of NOR. The use of different pH and inorganic anions also influenced NOR degradation. The degradation pathways of NOR were established and analyzed acute as well as chronic toxicities of NOR and its DPs.

Web URL: **https://www.sciencedirect.com/science/article/pii/S1010603022005287**

20. Khan, A., Niazi, M. B. K., Ansar, R., Jahan, Z., Javaid, F., Ahmad, R., ... & Bokhari, A. (2023). Thermochemical conversion of agricultural waste to hydrogen, methane, and biofuels: A review. Fuel, 351, 128947.

ABSTRACT:
With the depletion of fossil fuels, the energy crisis can now be visualized shortly. At the same time, waste production in various fields is also on the rise. This has led to a global waste management challenge. Agricultural wastes are produced in abundant amounts in various parts of the world, and they offer a potential substitute for fossil fuels. Agricultural wastes can be used to produce Methane, Hydrogen and biofuels along with various useful chemicals. This review provides insight into the composition of agricultural waste, the process of gasification, gasification agents, and challenges in the process. The fuels made from agricultural wastes, the pretreatment of agricultural waste and its challenges and future of energy production from agricultural waste are also discussed. The paper discusses in depth the reactions involved in the gasification process and the various types of gasifiers, their advantages and disadvantages. Energy production from agricultural waste is already being employed in few countries, but further research needs to make the processes more environmentally benign and eco-friendly. The logistics cost to transport the agricultural waste to biofuel plants is a major challenge that needs to be tackled. The feasibility of installing biofuel plants closer to agricultural fields is much better. For a smart usage of agricultural waste and to meet the sustainability criteria, it is necessary to integrate the available waste streams with local technical solutions.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0016236123015600**

21. Cao, Y., Sun, Y., Han, N., Li, X., Wang, Q., Sun, K., ... & Show, P. L. (2023). Novel highly active and selective CoNSC efficient ORR catalyst derived from in-situ egg gel pyrolysis. Fuel, 333, 126432.

ABSTRACT:

Exploring the influence of various heteroatoms on M N_x C and developing novel

synthetic M N C of strategies are great significance to improve the efficiency of continuable energy transformation and storage technologies. In this work, an economic and environmental in-situ doping synthesis scheme for extensible synthesis Co, N and S doped multiple porous-structure carbon (Co-NSEC) using egg gel as carbon precursor was reported. The Co-NSEC were certified to possess multiple porous structure, large surface area and uniform Co distribution. Moreover, systematic characterization results and electrochemical study revealed that thiophene sulfur could enhance Co-Nx oxygen reduction reaction (ORR) catalytic ability. The Co-NSEC catalysts exhibit excellent ORR performance akin to Pt/C (onset potential 0.947 V *vs* RHE, half-wave potential 0.842 V *vs* RHE, limiting current density 5.70 mA cm^{-2}) and better alcohol resistance and durability in alkaline solutions. The Co-NSEC electrocatalysts are promising as Pt replacement and are desired to be applied in the aspect of fuel cells.

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122032562

22. Ameen, I., Iqbal, S., Hussain, M., Alothman, A. A., Algahtani, H. A., Mushab, M. S. S., ... & Musaddiq, S. (2023). Ag, Au and ZrO2@ reduced graphene oxide nanocomposites; Pd free catalysis of suzuki-miyaura coupling reactions. Materials Research Express, 10(4), 045102.

ABSTRACT:

Suzuki coupling is a widely used, well-studied and versatile method in synthetic chemistry for development of C–C bonds where palladium-based catalysts have been used extensively in the reaction to date. We report a Suzuki-cross-coupling reaction for C–C bonds formation between aryl halides and phenylboronic acid by using Metal/metal oxide@Reduced graphene oxide nanocomposites being efficient, simple and cost-effective. In this work, plant mediated synthesis of silver, gold and zirconia nanoparticles doped Reduced Graphene Oxide nanocomposites is reported where 30 mg of each of the catalysts resulted in C-C bond formation achieving percentage yield comparable to palladium-based catalyst used as standard in series of reactions, attaining highest yield with silver based catalyst. The catalysts demonstrated high catalytic activity over three cycles of recycling with no loss. Bromoaryl and phenylboronic acid are coupled together by the increased surface area of the reduced graphene oxide substrate, which also exhibits enhanced reactivity toward other chemical reactions. XRD, FTIR and UV–vis analyses were used to describe the synthesized catalyst. Using the devised technique, various substituted aryl halides have been used successfully with modest to high yields of the desired biphenyls.

Web URL: https://iopscience.iop.org/article/10.1088/2053-1591/acce23/meta

23. Akhter, P., Nawaz, S., Shafiq, I., Nazir, A., Shafique, S., Jamil, F., ... & Hussain, M. (2023). Efficient visible light assisted photocatalysis using ZnO/TiO2 nanocomposites. Molecular Catalysis, 535, 112896.

ABSTRACT:
Photocatalysis is an effective green technology for breaking down organic dyes in aqueous environments. TiO_2 and ZnO have been widely explored for their use in photocatalysis because of their intrinsic properties, such as nontoxicity, stability, insolubility in water, high reactivity, and good photochemical properties. An effective binary composite ZnO/TiO_2 photocatalyst were synthesized using the sol-gel approach employing titanium tetraisopropoxide ($C_{12}H_{28}O_4Ti$) and zinc nitrate dihydrate [$Zn(NO_3)_2 \cdot 2H_2O$] as reagents. The photocatalytic effects of the produced samples were investigated using methylene blue when exposed to visible light. The size, shape, structure, phase composition, morphology, and optoelectronic properties of the materials were characterized using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and ultraviolet-visible spectroscopy (UV-Vis.) The parametric study revealed that an agitation rate of 1500 rpm, pH 4, 0.80 g/L catalyst loading, and 50 ppm of dye solution were the optimal conditions for the effective degradation reaction. Under the optimized reaction conditions, the novel ZnO/TiO_2 nanocomposite catalyst exhibited up to 96% dye degradation. A plausible reaction mechanism for the photocatalytic dye degradation reaction was also proposed. Moreover, the reusability/cyclic stability and kinetic study of the synthesized photocatalysts are highlighted, revealing that the material is sufficiently stable for commercialization, and the mechanism follows a pseudo-first-order kinetic model.

Web URL: https://www.sciencedirect.com/science/article/pii/S2468823122007829

24. Afsari, K., Emami, M. R. S., Zahmatkesh, S., Klemeš, J. J., & Bokhari, A. (2023). Optimizing the thermal performance of the thermosyphon heat pipe for energy saving with graphene oxide nanofluid. Energy, 274, 127422.

ABSTRACT:
A thermosyphon heat pipe (THP) involves a vacuum tube with a specific quantity of liquid. Due to its simplicity of design and structure, THP has many applications in heat recovery and renewable energy devices. Prior studies showed that using stable nanofluids can improve THPs' energy efficiency. In this evaluation, the effect of working fluid type, input heat, two types of surfactants, and nanoparticle concentration on the energy efficiency and thermal resistance of a THP was investigated and optimized. A magnetic stirrer and ultrasonic waves were used to create stability. Imaging and spectrophotometric analysis showed that graphene oxide (GO) nanofluid with SDS surfactant is more stable. The most notable decrease in thermal resistance at an input power of 100 W with GO nanofluids compared to distilled water at an F.R. of 50% was 12%. The highest decrease in the evaporator temperature section was achieved with GO and SDS surfactant at a weight ratio of 0.3% wt, equal to 12.3 °C. This was also confirmed by measuring

the contact angle. The highest percentage increase in thermal efficiency of THP with the mixture of GO nanoparticles and SDS surfactant in distilled water with 0.3 wt percent and input heat of 200 W was 18% compared to distilled water. In the optimum condition, the highest percentage increase in thermal efficiency of THP with the mixture of GO nanoparticles and SDS surfactant in distilled water with 0.3 wt percent and input heat of 200 W was 18% compared to distilled water.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360544223008162

25. Tan, X., Shen, Z., Bokhari, A., Ali, W., & Han, N. (2023). Effect of Co2O3 as sintering aid on perovskite BaCe0. 8Y0. 2O3-δ proton conductive membrane for hydrogen separation. International Journal of Hydrogen Energy.

ABSTRACT:

$BaCe_{0.8}Y_{0.2}O_{3-\delta}$ proton conductor powder was prepared by sol-gel method, and the effects of sintering temperature and sintering aids addition on the mechanical properties and hydrogen permeability of $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ proton conductor were investigated. XRD tests showed that when the addition of sintering aid Co_2O_3 reached 5%, the $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ proton conductor still showed a good perovskite phase. The sintering temperature of the sample with sintering aid is significantly lower than that of the blank sample. SEM shows that the addition of Co_2O_3, the proton conductor grains are closely arranged, the mechanical properties are increased, and the hydrogen permeability is significantly improved.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360319922054593

26. Maaz, M., Aslam, M., Yasin, M., Khan, A. L., Mushtaq, A., Fazal, T., ... & Kim, J. (2023). Macroalgal biochar synthesis and its implication on membrane fouling mitigation in fluidized bed membrane bioreactor for wastewater treatment. Chemosphere, 324, 138197.

ABSTRACT:

The intensification of biochar into fluidized bed membrane bioreactor was investigated to mitigate membrane fouling. Different biochars from algal biomass were produced and used as biomaterials for wastewater treatment. In this study, different macroalgal biochar was synthesized at different pyrolysis temperatures and characterized using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Brunauer Emmett-Teller (BET) and Fourier transform infrared spectroscopy (FTIR) techniques to implicate their effect on membrane fouling reduction in fluidized bed membrane bioreactor. The combined effect of macroalgal biochars and biocarriers with gas sparging was evaluated for fouling mitigation. Macroalgal biochar curtailed membrane fouling effectively at low gas sparging rate. Transmembrane pressure (TMP) was reduced to 0.053 bar; under the fluidization of biochar-650 and biocarriers with gas sparging; from 0.27 bar (gas sparging only). Combined effect of gas sparging, biocarriers and biochar-650 instigated 92.1% fouling reduction in comparative to gas sparging alone. Mechanical scouring driven by biocarriers could reduce fouling due to removing surface deposit of foulants from

membrane surface effectively and biochar can efficiently adsorb foulants because of its active functional groups resulting in reduction of colloidal fouling. The addition of divalent ions (Ca^{2+}) further enhanced the fouling reduction in fluidized bed membrane bioreactor.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653523004642

27. Alsaiari, M., Bokhari, A., Chuah, L. F., Mubashir, M., Harraz, F. A., Almohana, A. I., ... & Rizk, M. A. (2023). Synthesis of methyl esters from Hippophae rhamnoides via pilot scale hydrodynamic cavitation intensification reactor. Renewable Energy, 205, 238-247.

ABSTRACT:
The current research demonstrates the capability of hydrodynamic cavitation (HC) for the manufacture of ester sourcing *Hippophae rhamnoides* (HiRO) seed oil, which is non-edible in nature. According to the authors' best knowledge, the HC pilot developed assembly has not been put to use in any research pertaining to the manufacturing of biodiesel from HiRO triglycerides. The vast majority of the research indicates that optimising the system for the production of biodiesel based on a particular criterion, such as yield, can lead to only one portion of the research. In order to achieve maximum efficiency in the transesterification reaction, it is necessary to optimise not only the amount of output but also the cavitational parameters. The process of transesterification was initiated to overcome mass transfer resistance. In a pilot HC reactor, four novel geometries (orifices disk) cavities were explored. These cavities were helped along by a double diaphragm pump. It was shown that the mass transfer barrier between immiscible reactants can be decreased by increasing the interfacial area, and this effect was observed during the transesterification reaction, which is characterised by significant turbulence induced by cavitating bubbles. This was accomplished by increasing the surface area of the interface between the reactants. When compared to mechanical stirring, using an orifice plate with 21 holes that were 1 mm in diameter resulted in an eightfold increase in yield efficiency and a sixfold reduction in response reaction time at 2 bar inlet pressure. Utilising the hydrodynamic cavitation contributes to the procedure's reduced impact on the natural environment. In conclusion, the *Hippophae rhamnoides* oil methyl ester (HiROM) that was produced through the process of hydrodynamic cavitation was demonstrated to be both time and energy efficient. The characteristics of the methyl ester that was synthesised were in accordance with the requirements of both EN14214 and ASTM D6751.

Web URL: https://www.sciencedirect.com/science/article/pii/S0960148123000812

28. Ashraf, F., Ali, A., Park, J. H., Kim, J., Park, K., & Lim, H. J. (2023). In-situ measurement of secondary aerosol formation potential using a flow reactor: Livestock agricultural area. Atmospheric Environment, 301, 119695.

ABSTRACT:
Atmospheric ammonia (NH_3) is an important particulate matter (PM) precursor. The primary sources of ammonia in agriculture are livestock farming and synthetic fertilizers. Here, an oxidation flow reactor (OFR) was deployed in the vicinity of livestock farming during the

summer of 2020 and winter of 2021 to determine the extent of secondary aerosol formation. The OFR was run in a 1-h cycle of different aging times for the daytime and nighttime oxidants of OH and NO_3 radicals, respectively. The daytime reaction periods were 05:00–20:00 and 08:00–18:00, respectively, for summer and winter. Ambient and aged PM2.5 were characterized for secondary aerosol formation potential (AFP) using a time-of-flight aerosol chemical speciation monitor (ToF-ACSM). Ambient PM2.5 mean composition during summer was dominated in the order of nitrate (41%), organic matter (33%), ammonium (15%), and sulfate (11%). Secondary AFP was in the higher order, nitrate (71%), ammonium (20%), organic matter (8%), and sulfate (1%). A prominent effect of NH_3 was observed when the primary aerosol was aged at high NO_x and relative humidity (RH). Source apportionment revealed secondary organic aerosol (SOA)-dominant organic aerosols.

Web URL: https://www.sciencedirect.com/science/article/pii/S1352231023001218

29. Iqbal, M. S., Aslam, A. A., Iftikhar, R., Junaid, M., Imran, S. M., Nazir, M. S., ... & Ahmadipour, M. (2023). The potential of functionalized graphene-based composites for removing heavy metals and organic pollutants. Journal of Water Process Engineering, 53, 103809.

ABSTRACT:

The contamination of water sources with toxic pollutants such as heavy metals and organic compounds is a major environmental challenge in today's industrial era. These pollutants, which come from sources such as industries, agriculture, and domestic waste, could harm aquatic life and make the water unsafe for human use. Considering this issue in the combating environmental crises, removing pollutants from wastewater is one of the enduring environmental contests. Adsorption technology is an economical, fast, and efficient physicochemical method for eliminating both heavy metal and organic pollutants. In recent years, researchers have been exploring the use of functionalized graphene-based composite materials for the treatment of contaminated water, due to the large surface area, highly active surface, and exclusive physicochemical properties, which make them potential adsorbents with unique physicochemical properties. These materials, which could be developed using techniques such as chemical vapor deposition and chemical exfoliation, have been shown to effectively remove heavy metals and organic pollutants from water. This review article provides a thorough summary/critical appraisal of the published literature on graphene and its derivation based adsorbents for the removal of organic dyes and heavy metal ions pollutants from wastewater. The properties, synthesis methods, factor influence, mechanisms, and the performance of these substances are dissected. Finally, the research challenges, limitations, and future research studies are also discussed. Indeed, this review article will benefit the research community by getting substantial information on suitable techniques for synthesizing such adsorbents and utilizing them in water treatment and designing water treatment systems.

Web URL: https://www.sciencedirect.com/science/article/pii/S2214714423003288

30. Hussain, M. S., Ahmed, A., Yibin, L., Amin, M. N., Zahoor, T., Saleem, M. A., ... & Park, Y. (2023). Optimization analysis of the absorption-stabilization process for fluid catalytic cracking unit. Korean Journal of Chemical Engineering, 1-12.

ABSTRACT:
The absorption-stabilization process (ASP), an important part of petroleum refinery used in the end-use products of petroleum (such as stable gasoline, liquid petroleum gas, and dry gas), is energy-intensive and has low product quality. Aspen Plus process simulator was used for the development of the ASP process model. The developed process model was validated with the actual plant data. The validated model was used to optimize to minimize the cost of the ASP. This work shows that the optimization analysis of the ASP can further improve the product quality and reduce thermal energy consumption. In the new process, changing feeding parameters of supplementary absorption oil, stripping tower intermediate reboiler, and feeding position of stabilization tower reduced the C_3 contents of dry gas considerably and lowered the C_2 and lighter contents of LPG. Additionally, the new process saved 1.32 MW of thermal energy consumption compared with the existing process. The operating cost has been reduced from 10.921 million USD annually to 9.830 million USD per year. Furthermore, the cost-saving effect of this optimization is about 9.99% (1.091 million USD per year).

Web URL: https://link.springer.com/article/10.1007/s11814-023-1411-5

31. Riaz, I., Qamar, O. A., Jamil, F., Hussain, M., Inayat, A., Rocha-Meneses, L., ... & Park, Y. (2023). Comparative study of enhanced catalytic properties of clay-derived SiO2 catalysts for biodiesel production from waste chicken fat. Korean Journal of Chemical Engineering, 1-9.

ABSTRACT:
The use of biodiesel is a proactive measure that can be implemented to reduce emissions of greenhouse gases and other adverse environmental impacts. However, one of the major setbacks to biodiesel production is its relatively higher cost compared to petroleum diesel. The optimistic solution to this is valorization of biomasses like waste chicken fat (WCF) and clay for deriving non-edible oil and catalyst respectively. Herein, we report the synthesis of clay derived SiO_2 catalyst impregnated with SrO, Bi_2O_3, CuO and CaO. The developed catalysts were characterized by FTIR, XRD, and SEM. XRD studies confirmed the successful impregnation of active metallic oxide on SiO_2 support. Further, these catalysts were employed for biodiesel production from WCF, and SrO/SiO_2 was found to be most effective and efficient catalyst for biodiesel production from WCF. Hence, SrO/SiO_2 was adapted to optimize the different transesterification reaction parameters such as methanol to oil ratio, catalyst loading, reaction temperature and time. The optimized conditions for maximum biodiesel yield 98.9% were found to be 65 °C in 1 h with 12:1 methanol to oil ratio and 1 wt% catalyst loading. The biodiesel produced was also analyzed by GC-MS. The obtained biodiesel yield shows that clay can be a potential, and cost-effective, catalyst source to produce biodiesel from WCF.

Web URL: https://link.springer.com/article/10.1007/s11814-023-1467-2

32. Jrai, A. A., Al-Muhtaseb, A. A. H., Jamil, F., & Myint, M. T. Z. (2023). Green hydrocarbons fuel production from agricultural waste biomass in the presence of a novel heterogeneous catalyst. Biomass Conversion and Biorefinery, 1-14.

ABSTRACT:
Hydrocarbons (fuel) derived from agricultural waste biomass are potential alternatives, and these hydrocarbons are within range of jet fuel and diesel. In the current research work, date seeds are considered a feedstock for bio-oil (composed of oxygenated hydrocarbons) and is subjected to hydro-deoxygenation to produce green jet fuel and diesel. Hydro-deoxygenation is exothermic reaction and involves cracking for which a novel heterogeneous catalyst is synthesised. The heterogeneous catalyst consists of an acidic nature precursor derived from waste glass (SiO_2) and active metals (tungsten, nickel and palladium) to provide the acidic sites for better-desired product yield. The synthesised catalysts are characterised in detail by the following techniques X-ray diffraction analysis (XRD), Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDXS), Brunauer–Emmett–Teller (BET), Ammonia-Temperature programmed desorption (TPD) and X-ray Photoelectron Spectroscopy (XPS) and based on characterisation it is revealed that synthesised will be suitable for hydro-deoxygenation. The most appropriate combination of metal and precursor is Pd-SiO_2. Product oil's optimised degree of deoxygenation (DOD) is found to be 93.7% with the following parameters: temperature 340 °C, time 4 h and 4 wt.% of Pd on SiO_2. Further on, to prove the commercial viability of the catalyst, it was subjected to five consecutive experimental runs, and it was much active till 5^{th} run if treated before each run. Thus, it can be concluded that bio-oil source is agricultural waste, and for catalyst precursor waste glass is considered; so by considering these factors, the product oil produced has components which lie within the range of jet fuel and diesel, which can be economical as well as eco-friendly source of fuel.

Web URL: https://link.springer.com/article/10.1007/s13399-023-04076-1

33. Rashidi, A. R., Azelee, N. I. W., Zaidel, D. N. A., Chuah, L. F., Bokhari, A., El Enshasy, H. A., & Dailin, D. J. (2023). Unleashing the potential of xanthan: a comprehensive exploration of biosynthesis, production, and diverse applications. Bioprocess and biosystems engineering, 1-17.

ABSTRACT:
Employing aerobic fermentation, Gram-negative bacteria belonging to the genus Xanthomonas produce the high molecular weight natural heteropolysaccharide known as xanthan. It has various amounts of O-acetyl and pyruvyl residues together with D-glucosyl, D-mannosyl, and D-glucuronyl acid residues in a molar ratio of 2:2:1. The unique structure of xanthan allowed its various applications in a wide range of industries such as the food industry, pharmacology, cosmetics and enhanced oil recovery primarily in petroleum. The cultivation medium used in the manufacture of this biopolymer is critical. Many attempts have been undertaken to generate xanthan gum from agro-based and food industry wastes since producing xanthan gum from synthetic media is expensive. Optimal composition and processing parameters must also be considered to achieve an economically viable manufacturing process. There have been several attempts to adjust the nutrient content and feeding method, temperature, pH, agitation and the

use of antifoam in xanthan fermentations. Various modifications in technological approaches have been applied to enhance its physicochemical properties which showed significant improvement in the area studied. This review describes the biosynthesis production of xanthan with an emphasis on the importance of the upstream processes involving medium, processing parameters, and other factors that significantly contributed to the final application of this precious polysaccharide

Web URL: https://link.springer.com/article/10.1007/s00449-023-02870-9

34. Zhang, Y., Shen, B., Ahmad, M. S., Zhou, W., Khalid, R. R., Ibrahim, M., & Bokhari, A. (2023). A three-dimensional active biochar for sintering in steel industry and remove methylene blue by synergistic activation of H3PO4 and ZnCl2. Fuel, 336, 127079.

ABSTRACT:

In the context of treating waste with waste, the development of three-dimensional biochar that may be used for sintering in the steel sector as well as successfully removing methylene blue from waste water is effective. The biochar activated by H_3PO_4 alone (DCP), $ZnCl_2$ alone (DCZ) and H_3PO_4 cooperated with $ZnCl_2$ (DCM) were prepared to investigate the mechanism of the synergism of H_3PO_4 and $ZnCl_2$ at pyrolysis temperature 500 °C (selecting from 300 °C to 1000 °C). The SEM analysis indicates DCM possesses a stereoscopic porous network comparing agglomeration and stacking of the others, and the SEM and BET analysis indicate that DCM possesses a stereoscopic porous network and higher effective pore volume (VM/VT = 0.951) than DCP (VM/VT = 0.584) and DCZ (VM/VT = 0.812). EDS, XPS and FTIR analysis revealed that the surface heteroatom of P and Zn enhanced on DCM compared with that of DCP (P weight%=6.39 vs 3.26) and DCZ (Zn weight% = 5.93 vs 1.85) although the activator dosage was halved for DCM. The methylene blue isotherm adsorption curve of DCM fits well with Freundlich and Dual Langmuir adsorption isotherms, the adsorption kinetics is in line with the pseudo-second-order kinetic model. The results indicate that the adsorption process is based on a heterogeneous multilayer, that physisorption-chemisorption adsorption is the primary adsorption mechanism, and that the adsorption process is regulated by the combination of intra-particle and film diffusion. The DCM demonstrates to be a promising adsorbent for methylene blue removal, performing a high removal capacity at 576 mg/g. In this study, a feasible method to synergistically activate biochar from textile wastes was proposed, to deal with the removal of methylene

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122039035

35. Amin, N., Aslam, M., Yasin, M., Hossain, S., Shahid, M. K., Inayat, A., ... & Ghauri, M. (2023). Municipal solid waste treatment for bioenergy and resource production: Potential technologies, techno-economic-environmental aspects and implications of membrane-based recovery. Chemosphere, 138196.

ABSTRACT:

World estimated municipal solid waste generating at an alarming rate and its disposal is a severe concern of today's world. It is equivalent to 0.79 kg/d per person footprint and causing climate change; health hazards and other environmental issues which need attention on an urgent basis. Waste to energy (WTE) considers as an alternative renewable energy potential to recover energy from waste and reduce the global waste problems. WTE reduced the burden on fossil fuels for energy generation, waste volumes, environmental, and greenhouse gases emissions. This critical review aims to evaluate the source of solid waste generation and the possible routes of waste management such as biological landfill and thermal treatment (Incineration, pyrolysis, and gasification). Moreover, a comparative evaluation of different technologies was reviewed in terms of economic and environmental aspects along with their limitations and advantages. Critical literature revealed that gasification seemed to be the efficient route and environmentally sustainable. In addition, a framework for the gasification process, gasifier types, and selection of gasifiers for MSW was presented. The country-wise solutions recommendation was proposed for solid waste management with the least impact on the environment. Furthermore, key issues and potential perspectives that require urgent attention to facilitate global penetration are highlighted. Finally, practical implications of membrane and comparison membrane-based separation technology with other conventional technologies to recover bioenergy and resources were discussed. It is expected that this study will lead towards practical solution for future advancement in terms of economic and environmental concerns, and also provide economic feasibility and practical implications for global penetration.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653523004630

36. Ameen, M., Zafar, M., Ramadan, M. F., Ahmad, M., Makhkamov, T., Bokhari, A., ... & Show, P. L. (2023). Conversion of novel non-edible Bischofia javanica seed oil into methyl ester via recyclable zirconia-based phyto-nanocatalyst: A circular bioeconomy approach for eco-sustenance. Environmental Technology & Innovation, 30, 103101.

ABSTRACT:

The current study assesses *Bischofia javanica* Blume's potential as novel non-edible seed oil for environmentally benign biodiesel production using phyto-nanocatalyst, i.e., green nanoparticles (NPs) of zirconium oxide (ZrO_2) synthesized with aqueous leaf extract of the same plant *via* the biological method. Using response surface methods, the maximum yield (95.8 wt.%) was obtained at a 1:6 oil-to-methanol molar ratio, 2.5 wt.% catalyst loading, 70 °C reaction temperature and 2 h of reaction time. In addition, advanced analytical techniques such as Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM) with energy dispersive X-ray (EDX) were used to characterize green nanoparticles. Six peaks in the GC–MS spectrum were identified, showing the presence of six different methyl esters such as methyl palmitate, methyl linoleate, methyl oleate, methyl stearate, methyl linolenate and methyl 11-eicosenoate. In addition, ^{1}HNMR and ^{13}CNMR confirmed the high conversion yield of the esters group with distinct peaks at 3.649 ppm and 174.19 ppm. Biodiesel prepared from *Bischofia javanica* has fuel qualities that meet international standards. Fuel properties were found analogous to international standards viz. ASTM and EN. These include flash point (80 °C), density at 15 °C (0.8623 kg/L), kinematic viscosity (5.32 mm^2/s), cloud (−11 °C), pour point (−8 °C) and sulphur content of 0.00047 wt.%. The results indicate

that the green nanocatalyst and synthesized biodiesel from the *Bischofia javanica* appear to be highly reliable and cost-effective candidates for producing sustainable and eco-friendly biodiesel to overcome energy crises and climatic deteriorations, which would assist in the shift from a linear to a circular economy.

Web URL: **https://www.sciencedirect.com/science/article/pii/S2352186423000974**

37. Oyewo, A. T., Oluwole, O. O., Ajide, O. O., Omoniyi, T. E., Kim, H., Choi, Y. J., ... & Hussain, M. (2023). Optimization of the Factors Influencing Biodegradation and Thermal Stability of Banana Pseudo Stem Fibers in Nigeria. Journal of Natural Fibers, 20(1), 2181909.

ABSTRACT:
Lignocellulosic fibers, one of natural biopolymers, are derived from abundant banana pseudo stem (BPS) agricultural waste in different parts of Nigeria. In this study, the lignocellulosic fibers of three common banana cultivars, agbagba, paranta, and omini, were investigated to determine their chemical composition and mechanical properties. Furthermore, the experimental investigations were correlated with the corresponding Taguchi L9 orthogonal array design under three factors – fiber treatment, diameter, and cultivar type – to find the optimal factors that are pertinent to the desired biodegradation and thermal stability of the fibers. The optimization results indicated that the fiber treatment followed by diameter and the cultivar type was the most influential of the responses, respectively. However, increased cellulosic content led to higher tensile strength and modulus, while higher lignin corresponded to higher elasticity. Meanwhile, the predictions of the biodegradation and thermal stability derived from the Taguchi design via S/N ratio ANOVA and regression modeling correlated adequately with the corresponding experimental observations. Ultimately, the fibers with optimum factors were T3D1C1 and T3D1C3, where T3, D1, C1, and C3 denote that the associated fiber was treated with acetic acid, had a diameter of 60.77 μm, and belong to the cultivar type of agbagba and omini, respectively.

Web URL: **https://www.tandfonline.com/doi/full/10.1080/15440478.2023.2181909**

38. Chuah, L. F., Mokhtar, K., Ruslan, S. M. M., Bakar, A. A., Abdullah, M. A., Osman, N. H., ... & Show, P. L. (2023). Implementation of the energy efficiency existing ship index and carbon intensity indicator on domestic ship for marine environmental protection. Environmental research, 222, 115348.

ABSTRACT:
The International Maritime Organization has set a goal to achieve a 50% reduction of total annual greenhouse gas emission related to the international shipping by 2050 compared to the 2008 baseline emissions. Malaysia government has taken an initiative to investigate the assessment (cost-effectiveness) of this International Maritime Organization's short-term measure on Malaysian-registered domestic ships although this measure is only for international merchant ship. To achieve this, this paper collected the ship's data from the shipowners from 25 sample ships. Engine power limitation is the most cost-effective option, but low power limits can lead to

substantially increased sailing times. Based on cost-efficiency analysis, it creates for the purpose of compliance with the operational carbon intensity indicator. It found that even if it is possible to bring an asset back into service, it may not be possible to do so in a manner that generates a profit or complies with applicable regulations. In these situations, it may be more prudent to scrap the asset rather than run the risk of having it become a stranded asset. This is especially true for older tankers. Alternatives with lengthy payback periods are not desirable for the domestic tanker fleet that is already in operation.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0013935123001408**

39. Rashid, R., Mahboob, I., Shafique, S., Shafiq, I., Akhter, P., Park, Y. K., & Hussain, M. (2023). Exploring the environmental sustainability potential of the China-Pakistan economic corridor for Pakistan. Stochastic Environmental Research and Risk Assessment, 1-12.

ABSTRACT:
In 2013, China and Pakistan agreed to jointly build infrastructure and to generate power in order to support the development of Pakistan alongside the successful implementation of Belt and Road Initiative. The projects carried out under this agreement are collectively called the China-Pakistan Economic Corridor (CPEC), and the CPEC is anticipated to bring prosperity and peace to South Asia. Notably, the CPEC will improve the respective economies of both countries and the trade between them, establish a regional connection between these countries, solve their energy issues, increase their people's interactions, and develop their infrastructure, by the establishment of 2000 km-transportation infrastructure (pipelines, railways, and roads) between China (Kashgar) and Pakistan (Gwadar port) on the Arabian Sea, improving the China-Pakistan connectivity. However, Pakistan faces numerous potential eco-environmental vulnerabilities in implementing this multibillion-dollar CPEC. Although, the CPEC is a collection of game-changing infrastructure projects that will improve Pakistan's destiny and modernize it. The study also confirms that the people serving in different sectors of Pakistan have sufficient awareness and understanding of CPEC project. They are hopeful towards the advantages and execution of the CPEC project, indicating the effective strategies for supporting the sustainable development of Pakistan.

Web URL: **https://link.springer.com/article/10.1007/s00477-023-02474-5**

40. Batool, M., Abbas, M. A., Khan, I. A., Khan, M. Z., Saleem, M., Khan, A. U., ... & Ahmad, N. M. (2023). Response Surface Methodology Modeling Correlation of Polymer Composite Carbon Nanotubes/Chitosan Nanofiltration Membranes for Water Desalination. ACS ES&T Water, 3(5), 1406-1421.

ABSTRACT:
Quick population growth and worldwide industrialization is creating serious issues in accessing safe drinking water, which necessitates the exploration of operative and economical water

treatment methods. This study aims to develop chitosan and carbon nanotube (CNT)-incorporated nanofiltration polyethersulfone (PES) membranes via the phase inversion method that have effective salt rejection capability. Various membranes, i.e., pristine PES, PES─0.75 wt % chitosan, PES─0.1 wt % CNTs, and PES─0.1 wt % CNT/chitosan composites, were fabricated and characterized. The composition, surface texture, and cross-sectional microstructures of the synthesized membranes were investigated by using attenuated total reflection–Fourier-transform infrared spectroscopy, atomic-force microscopy, and scanning electron microscopy, respectively. The chitosan/MWNTs containing a PES membrane showed excellent water flux and salt rejection. This composite membrane registered a maximum water flux of 80.26 $L/m^2 \cdot h$ and ~95.5% salt rejection at 40 °C and 4 kg/cm^2 of feed water pressure, as validated by ANOVA analysis. Response surface methodology showed a complete fit for the experimental analysis. This study suggests that the designed membrane can be used in practice to treat brackish water.

Web URL:
https://pubs.acs.org/doi/full/10.1021/acsestwater.3c00107?casa_token=7GSxBmwexaoAAAAA%3AcDlYFqB-v5GGWdeuLjLcHR1Fmv-U41XojaeNj_F_pEKViIT94tPXn6vQTYJMIkX_YknsQSIuLSBQO2Y

41. Qamar, O. A., Jamil, F., Hussain, M., Ala'a, H., Inayat, A., Waris, A., ... & Park, Y. K. (2023). Feasibility-to-applications of value-added products from biomass: Current trends, challenges, and prospects. Chemical Engineering Journal, 454, 140240.

ABSTRACT:
The bio-oil obtained from thermochemical conversions of biomass (wood and agriculture waste, animal waste, solid waste etc.) can be an alternative to conventional liquid fossil fuels used in transportation or industrial sectors. However, bio-oil in its raw form is not of good quality as a fuel compared to conventional fossil derived fuels. In particular, bio-oil in its raw form has a low heating value, high oxygen and water contents, high viscosity and corrosive behavior. So, bio-oil needs to be upgraded for its direct use as a fuel. Meanwhile, the different kinds of valuable products can be derived from bio-oil: biofuels, biochemicals, and biopolymers when bio-oil is upgraded. The conversion of bio-oil into useful products has been the focus of numerous studies. Thus, it is crucial to study the research progress of this area to get the data needed to evaluate the viability of various processes for using bio-oil as feedstock in a comparative manner. Hence, this review article focuses on these value-added products and is twofold. The first fold explains the pyrolysis and hydrothermal liquefaction of biomass and compares the bio-oil properties obtained from both methods. Further, the second fold explains the key insights and respective state-of-the-art of generation techniques of value-added products from bio-oil in detail. In addition, value-added products from catalytic pyrolysis and their respective applications are also briefly discussed. Finally, the challenges and prospects of these techniques are presented. Based on this study, most of these technologies are still in the research and development (R&D) phase and cannot be scaled up due to technological limitations and cost intensive.

Web URL: https://www.sciencedirect.com/science/article/pii/S1385894722057205

42. Qamar, O. A., Jamil, F., Hussain, M., Bae, S., Inayat, A., Shah, N. S., ... & Park, Y. K. (2023). Advances in synthesis of TiO2 nanoparticles and their application to biodiesel production: A review. Chemical Engineering Journal, 460, 141734.

ABSTRACT:
Biodiesel is a strategic measure to mitigate greenhouse gas emissions and other negative environmental impacts in line with oxidation of fossil fuels. Alkali-catalysed transesterification is the conventional production protocols in biodiesel production due to its technical reliability in line with low maintenance cost. Nonetheless, alkali-catalysed biodiesel production required to use the refined lipid feedstock due to low tolerance against impurities. TiO_2 NPs have been widely employed as heterogeneous catalysts. Also, the use of TiO_2 NPs could be beneficial because TiO_2 adaptation in production of biodiesel could combine transesterification and esterification into a single process. Nonetheless, the general protocol in TiO_2 NPs synthesis could not circumvent to use hazardous/toxic chemicals leading to serious/acute health and environmental problems. Several studies have demonstrated that green synthesis of TiO_2 NPs using microorganisms and plants as alternate approaches can eliminate the problems associated with conventional methods without sacrificing the exceptional features of these nano materials. Hence, the main objective of this review is to offer fundamental insights and recent advances in green methods for producing TiO_2 NPs driven by various microorganisms and plants extract along with quick summary of physio-chemical methods. In particular, the TiO_2 NPs with reduced sizes (<60 nm) are possible to obtain using cost effective and eco-friendly green synthesis. Moreover, activity of TiO_2 NPs as catalysts and their effect on biodiesel selectivity is discussed using catalytic *trans*-esterification, esterification, and simultaneous *trans*-esterification and esterification processes. The combinations of TiO_2 NPs with other metallic and non-metallic materials are very selective and efficient for biodiesel production upto 98 %. This study appeals to research communities for adopting green synthesized TiO_2 NPs as nanocatalysts for eliminating economic and environmental issues.

Web URL: https://www.sciencedirect.com/science/article/pii/S1385894723004655

43. Ashfaq, M., Li, Y., Zubair, M., Ur Rehman, M. S., Sumrra, S. H., Nazar, M. F., ... & Sun, Q. (2023). Occurrence and risk evaluation of endocrine-disrupting chemicals in wastewater and surface water of Lahore, Pakistan. Environmental Geochemistry and Health, 1-15.

ABSTRACT:
The current study highlights the occurrence, spatial distribution, and risk assessment of 16 endocrine-disrupting chemicals (EDCs) including their transformation products (TPs) in the wastewater and surface water of Lahore, Pakistan, using solid-phase extraction followed by liquid chromatography–mass spectrometry and gas chromatography–mass spectrometry. The parent EDCs include bisphenol A (BPA), triclosan (TCS), triclocarban (TCC), estrone (E1), estradiol (E2), estriol (E3), ethinylestradiol (EE2), 4-*n*-octylphenol (4*n*-OP), and 4-*n*-nonylphenol (4*n*-NP). The TPs include two TPs each of BPA, TCC, and estrogens along with a TP of TCS. Most EDCs showed 100% detection frequency in the wastewater with highest median concentration of 1310 ng/L for E3. In the surface water, the highest median

concentration was, however, observed for BPA (54.6 ng/L). Spatial variations in terms of sum of concentration due to all EDCs and their TPs were observed at different sampling points which suggest contamination due to industrial waste from nearby industrial estate. Risk evaluation in terms of risk quotient (RQ) and estradiol equivalent factor (EEQ) showed that most of EDCs and their TPs could pose high risk and estrogenicity to the surrounding environment. From the results of the current study, it is observed that the environment of Pakistan is deteriorating and is potential risk for endocrine disruption. It is, therefore, recommended to take stringent measures to make it sustainable for current as well as for future generations.

Web URL: https://link.springer.com/article/10.1007/s10653-023-01527-6

44. Ali, F., Mehmood, S., Ashraf, A., Saleem, A., Younas, U., Ahmad, A., ... & Show, P. L. (2023). Ag–Cu Embedded SDS Nanoparticles for Efficient Removal of Toxic Organic Dyes from Water Medium. Industrial & Engineering Chemistry Research, 62(11), 4765-4777.

ABSTRACT:
Remediation of industrial water pollution is a trending subject to date for the researchers around the globe, due to its detrimental effects on human life as well as aquatic life. Azo dyes are the largest industrial water polluters in respect of volume while anthraquinone the second largest. Therefore, humongous considerations are being enumerated for the removal and decolorization of azo (AZ) dyestuff; however, for anthraquinone (AQ) dyes, these efforts are considerably minimal; although the later one poses a greater threat to environmental contamination, because of their reinforced structure. The current study is an effort toward this foremost issue. Chemical reduction synthesis of silver–copper (Ag–Cu) bimetallic nanoparticles (BNPs) was achieved using $NaBH_4$ as a reducing agent and sodium dodecyl sulfate (SDS) as a stabilizer. Characterization and morphological evaluation indicates two distinctive UV/vis absorption peaks for Ag and Cu. XRD studies for nanocomposite showed crystallite size of 8.96014 nm having an FCC structure. SEM with EDX confirmed the particle sizes of BNPs and SDS to be 17.14 and 114.56 nm, respectively. Potential catalytic activity and kinetic parameters of Ag–Cu BNPs@SDS were monitored against Methylene Blue (MB), Methyl Orange (MO), and eosin-y (EY). The percentage degradation recorded for the nanocatalyst against MO, MB, and EY was 95.21%, 98.57%, and 96.65%, respectively. This method can be adopted for the removal of multiple dyes from industrial effluent on a larger scale.

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45. Mahboob, I., Shafique, S., Shafiq, I., Akhter, P., Belousov, A. S., Show, P. L., ... & Hussain, M. (2023). Mesoporous LaVO4/MCM-48 nanocomposite with visible-light-driven photocatalytic degradation of phenol in wastewater. Environmental research, 218, 114983.

ABSTRACT:
Dearomatization through photocatalytic oxidation is a swiftly rising phenolic compounds removal technology that works at trifling operations requirements with a special

emphasis on the generation of nontoxic products. The study aims to develop a $LaVO_4$/MCM-48 nanocomposite that was prepared via a hydrothermally approach assisting the employment of an MCM-48 matrix, which was then utilized for phenol degradation processes. Various techniques including UV–Vis DRS, FTIR, PL, Raman, TEM, and BET analyses are employed to characterize the developed photocatalyst. The developed photocatalyst presented remarkable characteristics, especially increased light photon utilization, and reduced recombination rate leading to enhanced visible-light-driven photodegradation performance owing to the improved specific surface area, specific porosities, and <2 eV narrow energy bandgap. The $LaVO_4$/MCM-48 nanocomposite was experienced on aqueous phenol solution having 20 mg/L concentration under visible-light exposure, demonstrating exceptional performance in photodegradation up to 99.28%, comparatively higher than pure $LaVO_4$. The conducted kinetic measurements revealed good accordance with pseudo first-order. A possible reaction mechanism for photocatalytic degradation was also predicted. The as-synthesized $LaVO_4$/MCM-48 nanocomposite presented excellent stability and recyclability.

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46. Akhter, P., Shafiq, I., Ali, F., Hassan, F., Rehman, R., Shezad, N., ... & Park, Y. K. (2023). Montmorillonite-supported BiVO4 nanocomposite: synthesis, interface characteristics and enhanced photocatalytic activity for dye-contaminated wastewater. Journal of Industrial and Engineering Chemistry, 123, 238-247.

ABSTRACT:

Textile effluents may harm the human body as well as cause environmental pollution. For several decades researchers have been attempting to overcome this issue by introducing environmentally friendly technologies that degrade bulk dyes to mitigate hazards. Synthetic dyes are carcinogenic for humans as well as for other living organisms. Various techniques have been developed for the removal of these toxic compounds, advanced oxidation processes (AOPs) being the most used processes. In this study, Montmorillonite (MMT) supported $BiVO_4$ nanocomposite was prepared by the sol–gel method to degrade Brilliant Red 80 dye using photocatalysis. The $BiVO_4$/MMT composite was comprehensively characterized by several characterization techniques including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Raman, Photoluminescence spectroscopy (PL), and UV–Vis diffuse reflectance spectroscopy (UV–Vis-DRS). Interestingly, the composite material showed a narrow bandgap of 2.26 eV with strong light absorption in the visible range. A 1000-watt Xenon Lamp was used for activity performance measurement. The photocatalytic Brilliant Red 80 degradation activity was observed to be 99% degraded within 120 min of illumination compared to conventional $BiVO_4$ which showed around 80% degradation. Moreover, in this work, an acidic media was found to favor the degradation of Brilliant Red 80 dye.

Web URL: https://www.sciencedirect.com/science/article/pii/S1226086X23001818

47. Nawaz, S., Jamil, F., Akhter, P., Hussain, M., Jang, H., & Park, Y. K. (2022). Valorization of lignocellulosic rice husk producing biosilica and biofuels—A review. Journal of Physics: Energy, 5(1), 012003.

ABSTRACT:
Lignocellulosic biomass is an agricultural waste material abundantly produced in large quantities on earth. Rice husk (RH) is a type of lignocellulosic biomass and a huge byproduct of rice milling. Notably, the rice plant collects silica from the soil and stores the collected silica in the form of silicic acid inside the cellulose micro-compartments of the plant. Therefore, RH obtained from rice milling contains a significant quantity of amorphous silica, which can further be used for several other purposes. Furthermore, silica-rich RH can be employed as a raw material for the production of biofuels and biochars instantaneously via thermochemical processes such as pyrolysis and gasification. This article thoroughly explores a prospective method use to produce biosilica and energy from RH at the same time, which is currently under investigation. Moreover, this study also discusses current improvements in the synthesis of RH silica materials and their long-term use, particularly in energy and environmental functional materials. In terms of the environment, RH silica materials can remove heavy metals and organic pollutants in soil amendment, wastewater treatment, and gas purification via adsorption, catalysis, and integrative methods. In essence, there are numerous research and development obstacles to overcome in the production of biosilica and biofuels, respectively, from RH, and this review article highlights all of them.

Web URL: https://iopscience.iop.org/article/10.1088/2515-7655/aca5b4/meta

48. Oyewo, A. T., Oluwole, O. O., Ajide, O. O., Omoniyi, T. E., Akhter, P., Hamayun, M. H., ... & Hussain, M. (2023). Physico-chemical, thermal and micro-structural characterization of four common banana pseudo-stem fiber cultivars in Nigeria. Journal of Natural Fibers, 20(1), 2167031.

ABSTRACT:
This study explores Banana pseudo-stem fiber (BPSF) derived from BPF cultivars that are common in Nigeria. The four cultivars are known locally as Agbagba, Omini, Panbola, and Paranta. This study characterized these cultivars to gain insight into their physical, thermal and microstructural properties. The BPSFs were obtained after manual BPS retting and treated with a 2 wt. % sodium hydroxide solution to improve the fiber quality. Data from the characterization revealed the agbagba cultivar to give the highest percentage recovery (3%) and thermal stability at elevated temperatures with a residual char of 14%. The percentage of cellulose, lignin, hemicellulose, and ash content were determined by chemical composition analysis. FTIR spectroscopy showed a lower lignin and hemicellulose absorption band in the agbagba cultivar while scanning electron microscopy supported the FTIR results. Agabagba's crystallinity index (XRD) of 61.7% was higher than other cultivars, and X-ray fluorescence (XRF) and a biodegradation test also showed that only agbagba cultivar contained calcium and had the strongest resilience to microbial attack under simulated soil conditions. Agbagba BPSF may be a viable reinforcement in bio-fiber polymer composites needing high strength due to its balanced qualities that have been demonstrated in comparison to other cultivars.

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49. Javed, F., Zimmerman, W. B., Fazal, T., Hafeez, A., Mustafa, M., Rashid, N., & Rehman, F. (2023). Green synthesis of biodiesel from microalgae cultivated in industrial wastewater via microbubble induced esterification using bio-MOF-based heterogeneous catalyst. Chemical Engineering Research and Design, 189, 707-720.

ABSTRACT:
Conventional homogeneous catalysts are non-biodegradable, requiring complicated downstream separation, further diminishing the overall economics. In this paper, a new heterogeneous catalyst, a metal-organic framework modified by biomaterials (Bio-MOF), complexed with an ionic liquid ([HMIM][HSO_4]/Bio-MOF), has been synthesized and integrated with microbubble mediated mass transfer technology to overcome the challenges of low conversion. The ionic liquid 1-methylimidazole hydrogen sulfate provides enhanced reactivity, while the Bio-MOF provides more active sites for the reaction. Detailed kinetic analysis suggests the biodiesel production reaction occurs on the vapor/liquid (microalgae oil) interface. The results revealed a higher conversion of (molar ratio of oil: methanol =1: 15, catalyst loading = 0.5 wt% of MO, temperature = 70 ºC) 92 ± 4% was achieved in 30 min relative to acid-catalyzed biodiesel production. Along with higher reactivity and larger surface area provided by the catalysts, the unprecedented higher conversion and rate of reaction is attributed to the "local" excess of alcohol present at the interface and simultaneous removal of water from the reactor. The results of activation energy (7.9 kJ mol^{-1}), enthalpy (4.92 kJ mol^{-1}), entropy (−287 J mol^{-1}), and Gibbs free energy (103.58 kJ mol^{-1}) show that current process required less energy is required for biodiesel production. The catalyst was recycled seven times and showed high stability with little reduction in its activity over these seven runs. The study demonstrates that this newly developed catalyst provides a high reaction rate and conversion of biodiesel production from microalgae oil using a heterogeneous catalyst by integrating it with microbubble-mediated mass transfer.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0263876222006918**

50. Ali, F., Saleem, A., Batool, N., Khan, H. A., Rehman, R., Mehboob, R., ... & Hussain, M. (2023). Adsorption and kinetic studies of chromium (VI) removal using Ag2Cu2O3 nanoparticles. Zeitschrift für Physikalische Chemie, 237(4-5), 565-585.

ABSTRACT:
This study reports the removal of chromium (VI) from waste aqueous medium using disilver-dicopper oxide nanoparticles ($Ag_2Cu_2O_3$ NPs) as adsorbent, which were synthesized by adopting reduction route of chemical method and stabilized by emulsifier (sodium dodecyl sulfate [SDS]). Synthesized nanoparticles were further characterized using different analysis techniques such as UV–Vis for the detection of NPs via Λ_{max} and their point-zero charge (pzc) determination also done. Whereas, FTIR and XRD were done to determine the functional groups, crystal plane (tetragonal) and crystallite size (15.19 nm) of $Ag_2Cu_2O_3$ NPs respectively. SEM was used with EDX for morphology and elemental confirmation respectively. The synthesized nanoparticles were then employed for the adsorptive removal of chromium (VI) (Cr(VI)). Different parameters including pH, temperature, agitation time, adsorbate and adsorbent's concentration were also

studied. At optimized conditions, 0.5 g adsorbent, 40 ppm concentration of Cr(VI) solution along with 1 h agitation time were studied. Maximum observed adsorption and chromium removal efficiency was 96.66319 %. Four adsorption isotherms namely; Freundlich, Langmuir, Temkin and Harkins-Jeura were employed from which Freundlich adsorption model gives best fitting on experimental results. The kinetic modelling had shown that adsorption process follows second order kinetics. The thermodynamic studies of the adsorptive removal of Cr(VI) also evaluated. The $Ag_2Cu_2O_3$ NPs adsorbent's reusability were also determined. The study had proven that $Ag_2Cu_2O_3$ nanoparticles are efficient adsorbents for the removal of Cr(VI).

Web URL*:* https://www.degruyter.com/document/doi/10.1515/zpch-2022-0158/html

51. Asaad, S. M., Inayat, A., Jamil, F., Ghenai, C., & Shanableh, A. (2023). Optimization of Biodiesel Production from Waste Cooking Oil Using a Green Catalyst Prepared from Glass Waste and Animal Bones. Energies, 16(5), 2322.

ABSTRACT:

Biodiesel as a fuel has been shown to positively impact the environment; replacing or reducing the dependence on fossil fuels while providing a viable alternative. The use of waste oils, such as non-edible or used oils, can reduce competition with food, loss of resources, and the resulting higher prices. In this study, biodiesel was obtained by a transesterification reaction using used cooking oil from fast-food restaurants as the feedstock and catalysts from waste glass and animal bones as the silica and calcium oxide sources, respectively. Utilizing waste or non-edible oils for the production of biodiesel can lessen the competition with food sources while achieving environmental and ethical biofuel standards. Additionally, employing readily available waste oils and catalysts prepared from waste material is an economical and low-cost process compared to the use of conventional expensive feedstock and catalyst. The catalyst characterization for the prepared $CaO–SiO_2$ catalyst was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FT-IR). The reaction was optimized using the response surface methodology (RSM) with central composite design (CCD) by varying three parameters: methanol-to-oil ratio, catalyst weight fraction (wt%), and reaction time. The highest biodiesel yield obtained using Design Expert software was 92.3419% at the optimum conditions of a 14.83:1 methanol-to-oil molar ratio, 3.11 wt% catalyst, and 143 min reaction time. This proved that waste cooking oil with $CaO–SiO_2$ catalyst could be used in the transesterification process to produce a high yield of biodiesel, which was shown in the results obtained from the experimental runs.

Web URL*:* https://www.mdpi.com/1996-1073/16/5/2322

52. Ahmad, T., Iqbal, J., Bustam, M. A., Babar, M., Tahir, M. B., Sagir, M., ... & Show, P. L. (2023). Performance evaluation of phosphonium based deep eutectic solvents coated cerium oxide nanoparticles for CO2 capture. Environmental research, 222, 115314.

ABSTRACT:

The critical challenge being faced by our current modern society on a global scale is to reduce the surging effects of climate change and global warming, being caused by anthropogenic emissions of CO_2 in the environment. Present study reports the surface driven adsorption potential of deep eutectic solvents (DESs) surface functionalized cerium oxide nanoparticles (CeNPs) for low pressure CO_2 separation. The phosphonium based DESs were prepared using tetra butyl phosphoniumbromide as hydrogen bond acceptor (HBA) and 6 acids as hydrogen bond donors (HBDs). The as-developed DESs were characterized and employed for the surface functionalization of CeNPs with their subsequent utilization in adsorption-based CO_2 adsorption. The synthesis of as-prepared DESs was confirmed through FTIR measurements and absence of precipitates, revealed through visual observations. It was found that DES6 surface functionalized CeNPs demonstrated 27% higher adsorption performance for CO_2 capturing. On the contrary, DES3 coated CeNPs exhibited the least adsorption progress for CO_2 separation. The higher adsorption performance associated with DES6 coated CeNPs was due to enhanced surface affinity with CO_2 molecules that must have facilitated the mass transport characteristics and resulted an enhancement in CO_2 adsorption performance. Carboxylic groups could have generated an electric field inside the pores to attract more polarizable adsorbates including CO_2, are responsible for the relatively high values of CO2 adsorption. The quadruple movement of the CO_2 molecules with the electron-deficient and pluralizable nature led to the enhancement of the interactive forces between the CO_2 molecules and the CeNPs decorated with the carboxylic group hydrogen bond donor rich DES. The current findings may disclose the new research horizons and theoretical guidance for reduction in the environmental effects associated with uncontrolled CO_2 emission via employing DES surface coated potential CeNPs.

Web URL: https://www.sciencedirect.com/science/article/pii/S0013935123001068

53. Faisal, A., Javed, F., Hassan, M., Gorji, M. R., Akram, S., Rashid, N., & Rehman, F. (2023). Experimental and mathematical nonlinear rheological characterization of chicken fat oil-a sustainable feedstock for biodiesel. Biomass Conversion and Biorefinery, 13(8), 7043-7050.

ABSTRACT:

To meet the ever-increasing energy demands, significant amount of research is carried out to find environmentally friendly and renewable energy resources. Biodiesel production through animal fats such as chicken fat is considered as a lucrative option due to the presence of high concentration of triglycerides and free fatty acid content. Chicken fats also contain other organic compounds, which could affect the flow properties of biodiesel. Current study is focused on developing a robust model to analyze flow behavior/model of chicken fat oil with in-depth analysis of rheological properties such as shear stress and dynamic viscosity against shear rate and time respectively. The analysis is based on experimental results as well as mathematical model and found a good agreement between the model and the results. It was found that the viscosity of a feedstock is a critical parameter for biodiesel production. If viscosity changes drastically during chemical reaction, it leads to energy losses and ultimately increases the process cost. However, chicken fat results indicate that the viscosity of chicken fat slightly decreased in the application of the shear rate. Still, the change was very small, and viscosity restored to its

original value of 0.08 Pa.S, when stressed was removed. This indicate that the chicken fat oil exhibits the time-dependent non-Newtonian thixotropy fluid which leads to its potential for biodiesel production in the transport section

Web URL: https://link.springer.com/article/10.1007/s13399-021-01613-8

54. Kang, B. S., Farooq, A., Valizadeh, B., Lee, D., Seo, M. W., Jung, S. C., ... & Park, Y. K. (2024). Valorization of sewage sludge via air/steam gasification using activated carbon and biochar as catalysts. International Journal of Hydrogen Energy, 54, 284-293.

ABSTRACT:
The catalytic gasification of sewage sludge was explored using different catalyst particle sizes, bed temperatures, and gasifying agents. Activated carbon and sawdust biochar were used as catalysts in this study. The effects of the porosity of activated carbon on tar adsorption and cracking, and biochar containing alkali and alkaline earth metallic species (AAEMs), which can enhance gasification reactions, were investigated under different conditions. A catalyst bed temperature of 800 °C and particle size of 0.5–1.7 mm showed optimum conditions for increasing H_2 and CO content and decrease CO_2 fraction; however, a higher solid residue (~38 wt%) was also observed due to the high ash content in sewage sludge. Furthermore, the introduction of steam had a positive effect on the H_2 increment, owing to the presence of inherent AAEMs in the biochar, promoting water gas shift and hydrocarbon steam reforming reactions. The results of this study provide effective measures for using activated carbon and affordable biochar to enhance H_2 production with a parametric effect on the catalyst bed.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360319923019675

55. Hassan, S. U., Shafique, S., Palvasha, B. A., Saeed, M. H., Naqvi, S. A. R., Nadeem, S., ... & Park, Y. K. (2023). Photocatalytic degradation of industrial dye using hybrid filler impregnated poly-sulfone membrane and optimizing the catalytic performance using Box-Behnken design. Chemosphere, 313, 137418.

ABSTRACT:
Mixed Matrix Membranes have gained significant attention over the past few years due to their diverse applications, unique hybrid inorganic filler and polymeric properties. In this article, the impregnation of nano-hybrid filler (polyoxometalates (~POMs) encapsulated into the metal-organic framework (MOF) ~ PMOF) on the polysulfone membrane (~PSF) was done, resulting in a mix matrix membrane (~PMOF@PSF). The developed structure was characterized by Fourier transform infrared (FT-IR), powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and transmission electron microscopes (TEM). The results confirmed that the nano-hybrid filler was successfully fabricated on the surface of PSF. Different loading ratios of nano-hybrid filler (5%, 10%, 20%, 30%, and 40%) were used for impregnation. The study's objective was to enhance catalytic performance using

optimization curves designed using a three-level Box-Behnken Design (BBD) simulation. The photodegradation of Methylene Blue (~MB) was studied against PMOF@$PSF_{30\%}$ and was found to perform optimally when the concentration of catalyst, time of degradation, and temperature were 0.05–0.15 gm, 40–120 min, and 30–70 °C respectively. These experiments were replicated 15 times, and obtained results were further processed using a two-quadratic polynomial model to develop response surface methodology (RSM), which allowed for a functional relationship between the decolorization and experimental parameters. The optimal performance of the reaction mixture was calculated to be 0.15 gm for concentration, 70 °C for temperature, with an 80 min reaction time. Under these optimal conditions, the predicted decolorization of MB was 98.09%. Regression analysis with $R^2 > 0.99$ verified the fit of experimental results with predicted values. The PMOF@PSF $PSF_{30\%}$ demonstrated excellent reusability as its dye degradation properties were significantly unaffected after ten cycles.

Web URL*:* https://www.sciencedirect.com/science/article/pii/S004565352203911X

56. Sarwar, A., Razzaq, A., Zafar, M., Idrees, I., Rehman, F., & Kim, W. Y. (2023). Copper tungstate (CuWO4)/graphene quantum dots (GQDs) composite photocatalyst for enhanced degradation of phenol under visible light irradiation. Results in Physics, 45, 106253.

ABSTRACT:

Photocatalysis is one of the most preferred methods for the degradation of organic pollutants as it can lead to complete mineralization of organic pollutants employing sunlight as an energy source. Until so far enormous number of investigations have been done regarding the development of visible light responsive, stable, and cost effective photocatalysts. In the present work, owing to objectives mentioned above, an attempt was made to develop an efficient, cheaper, and visible light active composite photocatalyst consisting of moderate band gap, $CuWO_4$ with electron conductive graphene quantum dots. A series of photocatalysts was prepared by varying the amount of $CuWO_4$ while keeping the amount of GQDs fixed, and their activity was evaluated for the phenol degradation under visible light irradiation. The prepared photocatalysts were characterized by using X-ray diffraction (XRD), Scanning electron microscopy (SEM), Raman spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, and Photoluminescence (PL) for the evaluation of crystallinity, functional groups, and properties of charge carrier separation, respectively. The maximum efficiency of photodegradation of phenol simulated wastewater was achieved by sample 0.5GCW (optimized sample having 0.5 wt% of $CuWO_4$ with respect to fixed amount of GQDs), 53.41%, as compared to the pure $CuWO_4$ sample, which exhibited 19.08% efficiency. A possible mechanism for enhanced activity of $CuWO_4$ is proposed mainly due to efficient transfer of electrons from $CuWO_4$ to graphene quantum dots. The results show that the graphene quantum dots GQDs with the $CuWO_4$ significantly contributes to the improvement of photocatalytic performance.

Web URL: https://www.sciencedirect.com/science/article/pii/S2211379723000463

57. Muazzam, R., Hafeez, A., Uroos, M., Saeed, M., Rehman, F., & Muhammad, N. (2021). Plasma-based ozonolysis of lignin waste materials for the production of value-added chemicals. Biomass Conversion and Biorefinery, 1-17.

ABSTRACT:
Lignin is the second most abundant and underutilized heterogeneous biopolymer. Current methods, to depolymerize lignin into valuable fuels and chemicals, are facing challenges. The major barriers to the commercialization of these methods are expensive catalysts, energy cost, and difficulty in the separation of a complex mixture of products. Targeted synthesis of chemicals is aimed to get selective compounds that may offer ease of separation. Vanillin is the only chemical that is manufactured commercially from lignin. A facile, highly efficient, room temperature, and metal-free route to the targeted synthesis of vanillin using ozone produced by non-thermal plasma is presented in the current study. The recovered lignin has been characterized by FTIR, SEM/EDX, and HSQC for determining structural changes. The recovered lignin with a loose structure can be further converted into more valuable products. Operational conditions have been investigated to optimize vanillin production. Under optimum conditions, ~ 60% of vanillin (based on GC–MS analysis) was obtained with only 10 min of treatment. The product selectivity has been controlled by reaction time and reactant lignin concentration. The recovered lignin having a partially oxidized structure can be further subject to depolymerization to get more value from this biopolymer.

Web URL: https://link.springer.com/article/10.1007/s13399-021-01707-3

58. Sarwar, B., Khan, A. U., Aslam, M., Bokhari, A., Mubashir, M., Alothman, A. A., ... & Khoo, K. S. (2023). Comparative study of ZIF-8-materials for removal of hazardous compounds using physio-chemical remediation techniques. Environmental Research, 220, 115168.

ABSTRACT:
The inherent toxicity, mutagenicity and carcinogenicity of dyes that are discharged into aquatic ecosystems, harming the health of humans and animals. ZIF-8 based composites are regarded as good adsorbents for the breakdown of dyes in order to remove or degrade them. In the course of this research, metal-organic framework materials known as ZIF-8 and its two stable composites, ZIF-8/$BiCoO_3$ (MZBC) and ZIF-8/$BiYO_3$ (MZBY), were produced via a hydrothermal process and solvothermal process, respectively, for the dangerous Congo red (CR) dye removal from the solution in water using adsorption method. According to the findings, the most significant amount of CR dye that could be adsorbed is onto MZBC, followed by MZBY and ZIF-8. The pseudo-second-order kinetic model was used effectively to match the data for adsorption behavior and was confirmed using the Langmuir isotherm equation. There is a possibility that the pH and amount of adsorbent might influence the adsorption behavior of the adsorbents. According to the experiment results, the technique featured an endothermic adsorption reaction that spontaneously occurred. The higher adsorption capability of MZBC is because of the large surface area. This results in strong interactions between the functional groups on the surface of MZBC and CR dye molecules. In addition to the electrostatic connection between functional

group Zn–O–H on the surface of ZIF-8 in MZBC and the $–NH_2$ or SO_3 functional group areas in CR molecules, it also includes the strong π–π interaction of biphenyl rings.

Web URL*:* https://www.sciencedirect.com/science/article/pii/S0013935122024951

59. Amiri, M. K., Zaferani, S. P. G., Emami, M. R. S., Zahmatkesh, S., Pourhanasa, R., Namaghi, S. S., ... & Hajiaghaei-Keshteli, M. (2023). Multi-objective optimization of thermophysical properties GO powders-DW/EG Nf by RSM, NSGA-II, ANN, MLP and ML. Energy, 280, 128176.

ABSTRACT:

In this study, prediction, modeling, and optimization have been performed for four TPH properties of graphene oxide nano powder-deionized water/ethylene glycol nf, which is unique compared to other studies. Response surface methodology, artificial neural networks based on multiple layers of perceptron, and algorithms based on machine learning have been developed for prediction and modeling. RSM modeling resulted in coefficients of determination of 0.9984, 0.9986, 0.9995, and 0.9996 for TC (k), density (ρ), SHC (cp), and viscosity (μ), respectively. The highest prediction errors for RSM models were 0.3644%, 0.0374%, 2.049%, and 0.2296% for k, ρ, μ, and cp. A higher temperature and a higher WF of NPs increased the TC of the nf. The maximum MLP model error was 0.43%, 6.59%, 12.64%, and 1.04% for ρ, cp, μ, and k, respectively. TC and SHC were optimized using the NSGA-II algorithm. The NSGA-II procedure indicated the maximum k and cp occurred at the highest temperatures. The temperature must be kept at its maximum to reach the optimal stage. Also, it was proven that temperature is a much more significant parameter than the nanoparticle WF.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360544223015700

60. Asaad, S. M., Inayat, A., Rocha-Meneses, L., Jamil, F., Ghenai, C., & Shanableh, A. (2022). Prospective of response surface methodology as an optimization tool for biomass gasification process. Energies, 16(1), 40.

ABSTRACT:

The worldwide population growth and the technological advancements reported in the past few years have led to an increase in the production and consumption of energy. This has increased greenhouse gas (GHG) emissions, the primary driver of climate change. As a result, great attention has been paid to sustainable and green energy sources that can replace or reduce reliance on non-sustainable energy sources. Among the different types of renewable energy sources currently available, bioenergy has been reported as an attractive resource mainly due to its low cost and great availability. Bioenergy can be produced from different biomass sources and converted into biofuels or value-added products through thermochemical, biochemical, and chemical processes. Gasification is a thermochemical process commonly used for bioenergy production, and it is particularly attractive mainly due to its high efficiency. However, its performance is influenced by parameters such as type of feedstock, size of biomass particle, feed rate, type of reactor, temperature, pressure, equivalence ratio, steam to biomass ratio, gasification

agent, catalyst, and residence time. In this paper, the influence of different performance parameters in the gasification process is analyzed, and optimization and modelling techniques are proposed as a strategy for product yield enhancement.

Web URL*:* https://www.mdpi.com/1996-1073/16/1/40

61. Asaad, S. M., Inayat, A., Rocha-Meneses, L., Jamil, F., Ghenai, C., & Shanableh, A. (2022). Prospective of response surface methodology as an optimization tool for biomass gasification process. Energies, 16(1), 40.

ABSTRACT:

The worldwide population growth and the technological advancements reported in the past few years have led to an increase in the production and consumption of energy. This has increased greenhouse gas (GHG) emissions, the primary driver of climate change. As a result, great attention has been paid to sustainable and green energy sources that can replace or reduce reliance on non-sustainable energy sources. Among the different types of renewable energy sources currently available, bioenergy has been reported as an attractive resource mainly due to its low cost and great availability. Bioenergy can be produced from different biomass sources and converted into biofuels or value-added products through thermochemical, biochemical, and chemical processes. Gasification is a thermochemical process commonly used for bioenergy production, and it is particularly attractive mainly due to its high efficiency. However, its performance is influenced by parameters such as type of feedstock, size of biomass particle, feed rate, type of reactor, temperature, pressure, equivalence ratio, steam to biomass ratio, gasification agent, catalyst, and residence time. In this paper, the influence of different performance parameters in the gasification process is analyzed, and optimization and modelling techniques are proposed as a strategy for product yield enhancement.

Web URL: https://www.mdpi.com/1996-1073/16/1/40

62. Saif-ul-Allah, M. W., Khan, J., Ahmed, F., Hussain, A., Gillani, Z., Bazmi, A. A., & Khan, A. U. (2023). Convolutional neural network approach for reduction of nitrogen oxides emissions from pulverized coal-fired boiler in a power plant for sustainable environment. Computers & Chemical Engineering, 176, 108311.

ABSTRACT:

Coal-fired power plants are the main electric power source across many countries and cause major air pollution problems such as acid rain, smog, ozone depletion, and global warming. According to the best of the authors' knowledge, this is by far the first study that proposed 1-dimensional Convolutional Neural Network (1d-CNN) in combination with teaching learning self-study optimization (TLSO) algorithm for NOx emissions reduction by optimizing process input variables in a pulverized coal-fired power plant. The proposed model reduced the NOx emissions by 50.9%. In addition, the reduction experiment resulted in the early convergence superiority of the TSLO (130 s, 30th iteration) compared to genetic algorithm and Bayesian optimization. Based on the result, it is evident that combination of computationally inexpensive

1d-CNN and relatively fast converging TLSO could help process engineers reduce NOx emissions, which could ultimately contribute towards the goal of a sustainable environment.

Web URL: https://www.sciencedirect.com/science/article/pii/S0098135423001813

63. Iqbal, M. S., Yao, Z. B., Ruan, Y. K., Iftikhar, R., Hao, L. D., Robertson, A. W., ... & Sun, Z. Y. (2023). Single-atom catalysts for electrochemical N2 reduction to NH3. Rare Metals, 42(4), 1075-1097.

ABSTRACT:
The increasing demand for clean energy and growing concerns regarding environmental sustainability have led to greater attention devoted toward the production of clean fuels via green chemistry. In this respect, ammonia is a green alternative to fossil fuels and can serve as a clean energy source. There is now great interest in realizing the electrochemical reduction in atmospheric nitrogen (N_2) for cheap, environmentally friendly and reliable ammonia (NH_3) production worldwide. However, the robustness of the triple bond in N_2 and the low efficiency of candidate catalysts limit the utility of this conversion. Single atom catalysts have been found to be more effective than nanoparticles due to their unique properties, and thus have been studied extensively for the nitrogen reduction reaction. In this review, we have covered the recent advances in design and synthesis of noble metal and non-noble metal single atom catalysts for the electrochemical reduction in nitrogen during the years 2018–2022. The catalyst efficiencies, with reference to coordination preferences and theoretical studies have been discussed. Moreover, we also provide insights into the current challenges and some considerations for further future studies.

Web URL: https://link.springer.com/article/10.1007/s12598-022-02215-7

64. Istkhar, T., Hafeez, A., Javed, F., Fazal, T., Ahmad, F., Hussain, A., ... & Rehman, F. (2023). Intensification of esterification reaction microbubble mediated reactive distillation. Chemical Engineering and Processing-Process Intensification, 191, 109435.

ABSTRACT:
The current study is based on the microbubble mediated reactive distillation by converting conventional homogeneous liquid-liquid system into a heterogeneous vapour-liquid system. Microbubbles owing to their higher surface area to volume ratio provides better mass transfer as well increasing the conversion and rate of reaction. To prove the hypothesis, production of methyl acetate was investigated because of its industrial importance. The experimental plan was designed using Response Surface Methodology (RSM). It allowed analysing the effects of operational parameters simultaneously. The kinetics investigation demonstrated that the esterification reaction occurs, indeed, on the vapour liquid interface at the skin/surface of the bubble and follows pseudo-first order kinetics. The maximum conversion of the process was found to be 91% in 20 min which is significantly higher than any previous study. Furthermore, RSM and Gated Recurrent Unit (GRU) were employed to develop models to analyse the correlations among parameters and to predict the responses. The GRU produced higher

R^2 = 0.9981 as compared to R^2 = 0.9715 produced by RSM. The results depict that GRU model is more robust and reliable than Response Surface Methodology for parameter interaction study and response prediction.

Web URL: https://www.sciencedirect.com/science/article/pii/S0255270123001721

65. Suri, S. U. K., Majeed, M. K., & Ahmad, M. S. (2023). Simulation Analysis of Novel Integrated LNG Regasification-Organic Rankine Cycle and Anti-Sublimation Process to Generate Clean Energy. Energies, 16(6), 2824.

ABSTRACT:

Recently, the depletion of fossil fuel reserves and the harmful environmental effects caused by burning fossil fuels have signified the supreme importance of utilizing sustainable energy reserves such as geothermal and solar energies. The advancement of the Organic Rankine Cycle as a clean energy generation path by researchers has gained momentous demand for its commercialization. The sole Organic Rankine Cycle can produce a large amount of energy in contrast to other power production cycles. To make this clean energy recovery sustainable, liquefied natural gas cold energy can be utilized through regasification to integrate the Organic Rankine Cycle with the anti-sublimation carbon dioxide capture process, merging the biogas setup. Liquefied natural gas cold energy recovery has paramount importance with aspects of energy economy and environment preservation. Liquefied natural gas regasification in shell and tube heat exchangers poses a minimal freezing risk and is high duty. Anti-sublimation of biogas is an energy-intensive process. It can be materialized from liquefied natural gas cold energy implementation through the Organic Rankine Cycle by maintaining cryogenic temperatures there. In this situation, greenhouse gas emissions can be minimized. The simulation analysis is performed based on thermodynamic and techno-economic assessments of the poly-generation energy systems. It is proved to be useful in conducting by regulating different working fluids. The optimum electric power generated is 2492 MW. While the optimum net present value, energy efficiency, and exergy efficiency of this proposed energy system are 19.5, 57.13%, and 76.20%, respectively. The governmental authorities and environmental protection can benefit from this scientific research work to create an environmentally friendly atmosphere and energy for contemporary society.

Web URL: https://www.mdpi.com/1996-1073/16/6/2824

66. Aziz, T., Farid, A., Haq, F., Kiran, M., Ullah, N., Faisal, S., ... & Show, P. L. (2023). Role of silica-based porous cellulose nanocrystals in improving water absorption and mechanical properties. Environmental Research, 222, 115253.

ABSTRACT:

Epoxy resins are important thermosetting polymers. They are widely used in many applications i.e., adhesives, plastics, coatings and sealers. Epoxy molding compounds have attained dominance among common materials due to their excellent mechanical properties. The sol-gel simple method was applied to distinguish the impact on the colloidal time. The properties were obtained with silica-based fillers to enable their mechanical and thermal improvement. The work

which we have done here on epoxy-based nanocomposites was successfully modified. The purpose of this research was to look into the effects of cellulose nanocrystals (CNCs) on various properties and applications. CNCs have recently attracted a lot of interest in a variety of industries due to their high aspect ratio, and low density which makes them perfect candidates. Adding different amounts of silica-based nanocomposites to the epoxy system. Analyzed with different techniques such as Fourier-transformed infrared spectroscope (FTIR), thermogravimetric analysis (TGA) and scanning electronic microscopic (SEM) to investigate the morphological properties of modified composites. The various %-age of silica composite was prepared in the epoxy system. The 20% of silica was shown greater enhancement and improvement. They show a better result than D-400 epoxy. Increasing the silica, the transparency of the films decreased, because clustering appears. This shows that the broad use of CNCs in environmental engineering applications is possible, particularly for surface modification, which was evaluated for qualities such as absorption and chemical resistant behavior.

Web URL: https://www.sciencedirect.com/science/article/pii/S0013935123000452

67. Kim, J. Y., Lee, M., Oh, S., Kang, B., Yasin, M., & Chang, I. S. (2023). Acetogen and acetogenesis for biological syngas valorization. Bioresource Technology, 129368.

ABSTRACT:
The bioconversion of syngas using (homo)acetogens as biocatalysts shows promise as a viable option due to its higher selectivity and milder reaction conditions compared to thermochemical conversion. The current bioconversion process operates primarily to produce C2 chemicals (e.g., acetate and ethanol) with sufficient technology readiness levels (TRLs) in process engineering (as midstream) and product purification (as downstream). However, the economic feasibility of this process could be improved with greater biocatalytic options in the upstream phase. This review focuses on the Wood-Ljungdahl pathway (WLP) which is a biological syngas-utilization pathway, redox balance and ATP generation, suggesting that the use of a specific biocatalysts including *Eubacterium limosum* could be advantageous in syngas valorization. A pertinent strategy to mainly produce chemicals with a high degree of reduction is also provided with examples of flux control, mixed cultivation and mixotrophy. Finally, this article presents future direction of industrial utilization of syngas fermentation.

Web URL: https://www.sciencedirect.com/science/article/pii/S0960852423007940

68. Shehzad, A., Arslan, A., Rehman, F., Quazi, M. M., Butt, S. I., & Jamshaid, M. (2023). Corrosion behavior of copper, aluminium, and stainless steel 316L in chicken fat oil based biodiesel-diesel blends. Sustainable Energy Technologies and Assessments, 56, 103089.

ABSTRACT:
This study investigates the corrosion behavior of automotive materials in bio-based fuels. The Response Surface Methodology is employed to evaluate the corrosion rates of materials such as copper, aluminium, and stainless steel when they are exposed to chicken fat-based biodiesel.

Copper, aluminium, and stainless steel showed minimum corrosion rate at a blend percentage of 5.86 % when they were immersed for 920 h and maximum corrosion rate at blend percentage 34.14 % when these were immersed for 920 h. Meanwhile, the maximum corrosion rate was observed at a blend percentage of 34.14 % corresponding to the same immersion period. Optimum values indicated by RSM for copper and aluminium were noted at a blend percentage of 10 % and an immersion period of 720 h. Similarly, for stainless steel 316 l, these were 10.91 % and 754.44 h, respectively. Additionally, trials using the B100 for 920 h were conducted on copper, aluminium, and stainless steel 316 l, and the results showed considerably higher corrosion rates than those previously found. The surface morphology of the materials was investigated by X-ray Diffraction and Scanning Electron Microscopy, and it was revealed that copper was the most corrosive material in chicken fat oil-based biodiesel followed by aluminium and stainless steel 316 l.

Web URL: https://www.sciencedirect.com/science/article/pii/S2213138823000826

69. Nawaz, S., Jamil, F., Akhter, P., & Hussain, M. (2023). State-of-the-art novel catalyst synthesized from waste rice husk and eggshells for cleaner biodiesel production. Biofuels, 1-9.

ABSTRACT:
Biodiesel is a popular alternative useful fuel due to its low environmental impact. Herein, we developed new heterogeneous catalysts from waste-materials, rice husk and eggshells, and utilized for the biodiesel-making process. Apricot seeds are widely accessible around the world and are used as an oil feedstock to produce biodiesel, an ecologically beneficial fuel. Modified silica dioxide (obtained from rice husk) and calcium oxide (obtained from calcining eggshells) are used to make synthetic catalysts, with both materials being impregnated to increase their activity. Fourier transform infrared spectroscopy, X-ray diffraction, and scanning electron microscopy techniques utilized to evaluate the catalysts. Gas chromatography mass spectroscopy identified the components in biodiesel and raw apricot oil by retention duration and area peaks. The parametric research was performed to optimize the reaction conditions, the biodiesel synthesis is greatest at 55 to 65 °C, 90 min, 25 methanol to oil molar ratio, 3 wt.% catalyst loading, and 90% yield. The biodiesel's fuel characteristics and industry standards (ASTM6751 & EN14214) proved that it might be a renewable fuel. Furthermore, it discovered that the catalyst could be reprocessed up to five times without losing substantial activity. This research suggests that waste-derived catalysts can be used to make commercial biodiesel.

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70. Nawaz, S., Jamil, F., Akhter, P., & Hussain, M. (2023). State-of-the-art novel catalyst synthesized from waste rice husk and eggshells for cleaner biodiesel production. Biofuels, 1-9.

ABSTRACT:
Biodiesel is a popular alternative useful fuel due to its low environmental impact. Herein, we developed new heterogeneous catalysts from waste-materials, rice husk and eggshells, and utilized for the biodiesel-making process. Apricot seeds are widely accessible around the world and are used as an oil feedstock to produce biodiesel, an ecologically beneficial fuel. Modified silica dioxide (obtained from rice husk) and calcium oxide (obtained from calcining eggshells) are used to make synthetic catalysts, with both materials being impregnated to increase their activity. Fourier transform infrared spectroscopy, X-ray diffraction, and scanning electron microscopy techniques utilized to evaluate the catalysts. Gas chromatography mass spectroscopy identified the components in biodiesel and raw apricot oil by retention duration and area peaks. The parametric research was performed to optimize the reaction conditions, the biodiesel synthesis is greatest at 55 to 65 °C, 90 min, 25 methanol to oil molar ratio, 3 wt.% catalyst loading, and 90% yield. The biodiesel's fuel characteristics and industry standards (ASTM6751 & EN14214) proved that it might be a renewable fuel. Furthermore, it discovered that the catalyst could be reprocessed up to five times without losing substantial activity. This research suggests that waste-derived catalysts can be used to make commercial biodiesel.

Web URL: https://www.tandfonline.com/doi/full/10.1080/17597269.2023.2221878

71. Zaman, S. U., Mehdi, M. S., Umar, M., Rafiq, S., Zaman, M. K. U., Javed, M. D., ... & Tahir, N. (2023). Preparation of Ammonium Persulfate/Glycerol based Novel Deep Eutectic Solvent under controlled conditions; Characterizations, Physical properties. Journal of Molecular Structure, 1283, 135265.

ABSTRACT:
A mixture of pure compounds is a deep eutectic solvent (DES) if it has a low eutectic point temperature and remains liquid at operating temperatures within a specific composition range. They are prepared by a combination of salt with hydrogen bond donor (HBD) moiety to some definite molar ratio. In the current study, a novel deep eutectic solvent was prepared by combining ammonium persulfate and glycerol in a 1:1.2 molar ratio using a discrete ramp input temperature response to prevent an uncontrolled reaction that could result in the emission of smoke and potential bursting. The affinity of ammonium persulfate for mixing with other HBDs was not significant. Moreover, the bonding behavior of the novel deep eutectic solvent was determined through FTIR spectroscopic analysis, which confirmed the physiochemical combination of its constituents and indicated the successful preparation of the DES, as evidenced by the significant shift of its characteristic peaks. The photoluminescence spectroscopic study was carried out to get insight about the electronic properties of the DES sample. The relationship between electrical conductivity rise with temperature was studied via a calibrated digital hand-held conductivity meter. The physical properties such as density, viscosity, surface tension, and freezing point of the immaculate DES at different temperatures were also reported. The variation

in physical characteristics allowed the prepared DES to be appropriate for miscellaneous applications.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0022286023003629**

72. Arshad, S., Ahmad, M., Munir, M., Sultana, S., Zafar, M., Dawood, S., ... & Show, P. L. (2023). Assessing the potential of green CdO2 nano-catalyst for the synthesis of biodiesel using non-edible seed oil of Malabar Ebony. Fuel, 333, 126492.

ABSTRACT:
Sustainable biodiesel synthesis from waste, toxic and non-edible oil seeds give a sustainable opportunity to combat energy crises and environmental depreciation. A new non-edible oil of *Diospyros malabarica* (Malabar Ebony) was analyzed for the synthesis of eco-friendly biodiesel using newly synthesized green nanoparticles (NPs) of Cadmium oxide (CdO_2) prepared from leaf extract of *Buxus papillosa* via biological method followed by in situ wet impregnation approach. The highest fatty acid methyl ester (FAME) yield of 94 wt% was attained through the process of transesterification at ideal experimental conditions i.e., 1:9 M ratio of oil to methanol, catalyst loading 0.5 wt%, experiment duration 180 min and reaction temperature of 90 °C. Optimize biodiesel yield from *Diospyros malabarica* using response surface methodology was also applied. Scanning electron microscopy (SEM), energy dispersive X-ray (EDX), thermogravimetric analysis and X-ray diffraction (XRD) were utilized for the characterization of newly synthesized CdO_2 NPs. The findings obtained from SEM revealed that CdO_2 NPs were cubic in shape. The size of CdO_2 NPs was 45 nm, which obtained from XRD analysis. EDX analysis showed 83.72 % cadmium composition. In thermogravimetric analysis, 5.2 % thermal degradation was observed which revealed that CdO_2 NPs have strong thermal stability. The production of FAME was confirmed by using gas chromatography-mass spectroscopy (GC–MS), nuclear magnetic resonanceand Fourier transform infrared spectroscopy techniques. 9-Octadecenoic acid is the key fatty acid with the highest abundance in the GC–MS spectrum. This study revealed that inedible oil seed of *Diospyros malabarica* and newly synthesized green NPs of CdO_2 has the highest potential to be used as highly reliable cost-effective and sustainable entrants for synthesizing eco-friendly diesel which is ultimately open up the avenue for further research in the exploration and application of economical feedstock for biodiesel industry at a larger scale.

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236122033166

73. Inayat, A., Tariq, R., Khan, Z., Ghenai, C., Kamil, M., Jamil, F., & Shanableh, A. (2020). A comprehensive review on advanced thermochemical processes for bio-hydrogen production via microwave and plasma technologies. Biomass Conversion and Biorefinery, 1-10.

ABSTRACT:
Substantial advances in research, thriving use, and further product recovery contribute to improvements and variations in current biomass processing thermochemical processes. This

study offers a summary of the concepts, methods, benefits, and demerits of biomass thermochemical conversions such as pyrolysis and gasification using microwave and plasma technologies for bio-hydrogen production. This article also offers a comprehensive overview of the evolving biogas for bio-hydrogen production. These technologies generate up to 95% bio-hydrogen and can process a wide variety of biomass and waste. The current study also includes assessing the overall description of the microwave plasma cycle and the effect of several operational parameters on H_2 performance. This extensive knowledge will help potential researchers to interlink with industry to make feasible, sustainable hydrogen production.

Web URL: https://link.springer.com/article/10.1007/s13399-020-01175-1

74. Inayat, A., Jamil, F., Ahmed, S. F., Ayoub, M., Abdul, P. M., Aslam, M., ... & Mustafa, A. (2023). Thermal degradation characteristics, kinetic and thermodynamic analyses of date palm surface fibers at different heating rates. Fuel, 335, 127076.

ABSTRACT:

The potential of the least-exploited date pam waste was presented as feedstock for bio-oil production. The surface fibers of the date palm are widely available as waste material in the Gulf region, the Middle East, and Africa. Chemical composition analysis and physiochemical characterization showed that surface fibers are valuable feedstock for energy production. Surface fibers were analyzed thermogravimetrically at different heating rates (10, 20, and 30 °C /min) in an inert atmosphere. Decomposition was carried out in three stages: dehydration, devolatilization, and solid combustion. Kinetic analysis was performed on the devolatilization region using the Coats–Redfern model–fitting method using twenty–one reaction mechanisms from four different solid-state reaction mechanisms. Two diffusion models: one–way transport ($g(x) = \alpha^2$) and Valensi equation ($g(x) = \alpha+(1-\alpha) \times \ln(1-\alpha)$) showed the highest regression coefficient (R^2) with the experimental data. The activation energy (��) and the pre-exponential factor (A) was estimated to be 91.40 kJ/mol and 1.59×10^3 –29.39×10^3 min^{-1}, respectively. The kinetic parameters were found to be dependent on the heating rate. The surface fibers' thermodynamic parameters ΔH, ΔG, and ΔS were 80–97, 151–164, and −0.17- −0.18 kJ/mol, respectively. This indicates that the pyrolysis of surface fibers is endothermal and not spontaneous. Since there is not much experimental work on the pyrolysis of surface fibers available in the literature, the reported results are crucial for designing the pyrolysis process.

Web URL: https://www.sciencedirect.com/science/article/pii/S001623612203900X

75. Mahboob, I., Shafiq, I., Shafique, S., Akhter, P., Munir, M., Saeed, M., ... & Hussain, M. (2023). Porous Ag3VO4/KIT-6 composite: Synthesis, characterization and enhanced photocatalytic performance for degradation of Congo Red. Chemosphere, 311, 137180.

ABSTRACT:

Novel Ag_3VO_4/KIT-6 nanocomposite photocatalyst has been successfully fabricated by a newly-designed simple hard-template induction process, in which the particles of Ag_3VO_4 were grown on the KIT-6 surface and inside the porous framework of the silica matrix. The developed porous

framework nanocomposite was characterized by several techniques including N_2-Physiosorption analysis. The obtained nanocomposite revealed a high surface area (273.86 m^2/g) along with the possession of monoclinic Ag_3VO_4, which is highly responsive to visible light (with distinct intensity at about 700 nm). The UV–Vis DRS reveals that the Ag_3VO_4/KIT-6 photocatalyst bears a bandgap of 2.29 eV which confirms that the material has a good visible light response. The synthesized nanocomposite was tested for its superior physicochemical properties by evaluating its degradation efficiency for Congo Red (CR). The novel composite exhibited superior degradation capability of CR, reaching up to 96.49%, which was around three times the pure Ag_3VO_4. The detailed kinetic study revealed that the as-prepared material followed a pseudo first order kinetic model for the CR degradation. The study includes a comprehensive parametric study for the formulation of the optimized reaction conditions for photocatalytic reactions. The commercial applicability of the composite material was investigated by a regeneration and recyclability test, which revealed extraordinary results. Furthermore, the possible degradation pathway for CR was also proposed.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653522036736

76. Aziz, T., Haq, F., Farid, A., Kiran, M., Faisal, S., Ullah, A., ... & Show, P. L. (2023). Challenges associated with cellulose composite material: Facet engineering and prospective. Environmental Research, 223, 115429.

ABSTRACT:
Cellulose is the most abundant polysaccharide on earth. It has a large number of desirable properties. Its low toxicity makes it more useful for a variety of applications. Nowadays, its composites are used in most engineering fields. Composite consists of a polymer matrix and use as a reinforcing material. By reducing the cost of traditional fibers, it has an increasing demand for environment-friendly purposes. The use of these types of composites is inherent in moisture absorption with hindered natural fibers. This determines the reduction of polymer composite material. By appropriate chemical surface treatment of cellulose composite materials, the effect could be diminished. The most modern and advanced techniques and methods for the preparation of cellulose and polymer composites are discussed here. Cellulosic composites show a reinforcing effect on the polymer matrix as pointed out by mechanical characterization. Researchers tried their hard work to study different ways of converting various agricultural by-products into useful eco-friendly polymer composites for sustainable production. Cellulose plays building blocks, that are critical for polymer products and their engineering applications. The most common method used to prepare composites is *in-situ* polymerization. This help to increase the yields of cellulosic composites with a significant enhancement in thermal stability and mechanical properties. Recently, cellulose composites used as enhancing the incorporation of inorganic materials in multi-functional properties. Furthermore, we have summarized in this review the potential applications of cellulose composites in different fields like packaging, aerogels, hydrogels, and fibers.

Web URL: https://www.sciencedirect.com/science/article/pii/S0013935123002219

77. Maqbool, M. A., Khan, J., Hamayun, M. H., Ahmed, F., & Hussain, M. (2023). Optimal retrofitting of MCH-Toluene dehydrogenation system: Energy and technoeconomic analysis. Energy Conversion and Management, 286, 117049.

ABSTRACT:

The rapid consumption of fossil fuels and the decline of conventional energy sources are diverting the world energy demand towards clean and sustainable energy. Hydrogen gas is under consideration for past few years as the clean energy source. But hydrogen itself is facing storage and transportation issues, and liquid organic hydrogen carriers (LOHCs) are the viable potential option to meet this need of the hour. Methylcyclohexane-toluene (MCH-Toluene) is one of the most appropriate LOHCs as compared to any other. Several studies in the past have focused mainly on the sensitivity analysis or the effect of catalysts on different operational parameters such as conversion of the reaction, but according to the best of authors' knowledge, the MCH-Toluene dehydrogenation system has not yet been rigorously optimized to reduce the total energy demand of the system. This study first unfolds the process configuration modification of the MCH-Toluene dehydrogenation system for its retrofitting based on heat integration. This retrofitted MCH-Toluene dehydrogenation system is then rigorously optimized to present an optimal process with respect to energy demand. A fast converging and consistent optimization approach named teaching learning self-study algorithm is used to achieve maximum potential thermodynamic performance of the proposed retrofit. The optimization of the system results in the total energy demand of the system reduced by the 6.07% as compared to the base case. The economic evaluation shows that the total investment required for MCH-toluene system and the total annual operating cost are reduced from $ 2.67 million and $ 2.42 million in the base case to $ 1.36 million and $ 1.6 million in this case, respectively. The levelized cost of hydrogen product is decreased from 1.6 $/kg H_2 in the base case to 1.08 $/kg H_2 in this study. As this method is reliable and efficient to reduce the total energy demand of the system, it could be more beneficial and helpful for the process engineers in the future.

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DEPARTMENT OF CHEMESTRY

1. Allangawi, A., Gilani, M. A., Ayub, K., & Mahmood, T. (2023). First row transition metal doped B12P12 and Al12P12 nanocages as excellent single atom catalysts for the hydrogen evolution reaction. International Journal of Hydrogen Energy, 48(44), 16663-16677.

ABSTRACT:
The hydrogen evolution reaction (HER) is a promising process to produce high purity hydrogen gas. However, the overpotential of this reaction hinders its practical applications. Single atom catalysts (SACs) are recently investigated by the scientific community to facilitate the HER. Herein, we studied the doping of late first-row transition metals on the $B_{12}P_{12}$ and $Al_{12}P_{12}$ nano-cages as SACs via density functional theory (DFT) calculations. Results show that all transition metals are chemisorbed on the support, with interaction energies ranging from −0.65 to −3.85 eV. The calculated Gibbs free energies of hydrogen evolution are −0.01, −0.06 and −0.20 eV for $Ni@Al_{12}P_{12}$, $Ni@B_{12}P_{12}$, and $Co@B_{12}P_{12}$, respectively, which are close to the optimum value of 0.00 eV, and comparable to the highly active Pt-based catalysts in literature. Our results indicate that the designed $Ni@Al_{12}P_{12}$, $Ni@B_{12}P_{12}$, and $Co@B_{12}P_{12}$ SACs are excellent candidates as noble metal-free, sufficiently stable, and highly efficient electrocatalysts for HER.

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2. Kosar, N., Zari, L., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Giant NLO response and ultraviolet transparency of superalakalis decorated C6O6Li6 complexes; a DFT perspective. Physica Scripta, 98(6), 065909.

ABSTRACT:
Materials having nonlinear optical (NLO) properties are the demand of optics and optoelectronics fields because of their widespread applications. Keeping in view the applications of NLO materials, some new superalkalis doped $C_6O_6Li_6$ complexes are introduced in this study having remarkable NLO response. Thermodynamic stability of nonlinear optical materials (NLO) is prime requirement of experimentalists for practical applications. All the considered complexes have high thermodynamic stability. Furthermore, these superalkali doped complexes reveal fabulous electronic properties. Superalkalis shift their outer shell electrons towards the $C_6O_6Li_6$ nanocluster, which act as diffuse excess

electrons. The HOMO-LUMO gaps (H-L E_{gap}) of superalkali doped complexes are effectively reduced due to shifting of electrons that reveals their conducting properties. NBO charge analysis confirmed electron charge transfer from superalkalis to $C_6O_6Li_6$ surface. Linear and NLO properties of these complexes are estimated from first order polarizability (α_o) and hyperpolarizability (β_o) parameters. Among all complexes, $C_6O_6Li_6.K_3O$ has the highest first hyperpolarizability ($\beta_o = 6.02 \times 10^5$ au). TD-DFT analysis confirmed the ultraviolet transparency of doped complexes. Two level model is used to rationalize the trend of first hyperpolarizability and the internal factors responsible for the enhancement of NLO response.

Web URL: https://iopscience.iop.org/article/10.1088/1402-4896/accf4b/meta

3. Bano, R., Ayub, K., Mahmood, T., Arshad, M., Sharif, A., Tabassum, S., & Gilani, M. A. (2023). Diamondoid as potential nonlinear optical material by superalkali doping: a first principles study. Diamond and Related Materials, 135, 109826.

ABSTRACT:

Adamantane ($C_{10}H_{16}$), the smallest diamondoid molecule, has sparked considerable scientific interest due to its symmetric, single cage-shaped structure. In the current work, the geometric, electronic, and nonlinear optical responses of Li_3O, Na_3O and K_3O clusters doped adamantanes have been investigated via DFT simulations. The calculated values of interaction energies (−5.50 to −6.91 kcal/mol) and vertical ionization energies (3.01–3.56 eV) reflected that the designed M_3O-Ada complexes are thermodynamically and chemically stable. Charge transfer is probed through natural population analysis and the highest charge transfer (0.038 |e|) is observed for K_3O-Ada complex. The electride nature of M_3O-Ada complexes is confirmed through their electron density distribution and their energy gaps (2.19–3.06 eV) are reduced significantly. Interestingly, the absorption maxima (1387–1629 nm) of M_3O-Ada electrides fall in the near infrared region. The highest first and second hyperpolarizability values of 5.9×10^5 au and 2.6×10^8 au are observed for K_3O-Ada electride. The maximum hyper-Rayleigh scattering and second harmonic generation values of 1.3×10^7 au and 6.5×10^6 au are obtained at 1907 nm whereas the electro-optical Pockel's effect (6.5×10^6 au) is maximum at 1064 nm. Moreover, the dynamic second hyperpolarizability co-efficients (EOKE, EFISHG) are also computed at varying wavelengths. The M_3O-Ada electrides exhibit the maximum nonlinear refractive index n_2 of 1.9×10^{-7} cm^2 W^{-1} at 1064 nm. This study will pave the way to the designing of stable superalkali doped diamondoids with enhanced NLO response.

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4. Kosar, N., Wajid, S., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). First, second and third order NLO response of alkaline earth metals doped C6O6Li6 organometallic complexes. Chemical Physics, 570, 111894.

ABSTRACT:
The geometric, electronic, linear and nonlinear (NLO) properties of pure $C_6O_6Li_6$ and alkaline earth metals (AEM) doped $C_6O_6Li_6$ organometallics are studied through quantum chemical methods. Interaction (E_{int}) and vertical ionization energies illustrate the thermodynamic and electronic stabilities of considered AEM@$C_6O_6Li_6$ organometallic complexes, respectively. The highest interaction energy value is noticed for Ca@$C_6O_6Li_6$ complex (–22.78 kcal/mol). After doping of alkaline earth metals, HOMO-LUMO energy gap (H-L Egap) is remarkably reduced. The variation in H-L Egap indicates the conductive properties of these complexes which occur due to transfer of electrons from the alkaline earth metals to the $C_6O_6Li_6$ surface or *vice versa*. The electronic density shifting is also supported by natural bond orbital (NBO) charge and molecular orbitals analyses. UV–VIS analysis is used to confirm the electronic excitations. These organometallics show deep ultra-violet transparency below 200 nm which justifies their application in future laser devices. A noticeable NLO response is observed for these organometallics which is confirmed from the static first order hyperpolarizability (up to 1.90×10^4 au) and second order hyperpolarizability (up to 7.11×10^6 au) along with higher refractive index (up to 1.68×10^{-12} au) at 532 nm. The hyperpolarizability values are further enhanced at dynamic frequencies and these are increased up to 5.82×10^{10} au. These results illustrate the use of these organometallics in optical technologies for achieving better dc-Kerr effect and second harmonic generation effects.

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5. Asif, M., Sajid, H., Qureshi, S., Gilani, M. A., Mahmood, T., & Ayub, K. (2023). Boron-rich triphenylene COF based electrides having excellent nonlinear optical activity. Materials Science in Semiconductor Processing, 160, 107468.

ABSTRACT:
The desirability of the high nonlinear response of two-dimensional (2D) materials for electronics and optoelectronic devices drove us to investigate the nonlinear optical (NLO) behavior of alkali metal atom (AA) doped lithiated boron-containing hexahydroxy-triphenylene (LiBHHTP). In this context, the geometric, electronic, optical, and NLO properties are investigated. The doped AA atoms including Li, Na, and K preferably interact via the oxygen atoms of the LiBHHTP surface. The stability of the doped complexes is revealed by the interaction energies (E_{int}), which are −22.90, −16.10, and −16.52 kcal/mol for Li@LiBHHTP, Na@LiBHHTP, and K@LiBHHTP complexes, respectively. The alterations in the electronic behavior of LiBHHTP are observed upon doping with alkali atoms via Frontier Molecular Orbital (FMO), Natural Bond Orbital (NBO), and the Density of State (DOS) analyses. The FMO analysis reveals that these complexes are electride in nature with absorption transparency in the UV–Vis range. Finally, the NLO behavior of designed complexes is evaluated through static and dynamic hyperpolarizabilities. Among reported complexes, K@LiBHHTP exhibits significantly large static hyperpolarizability (β_o), 2.24×10^5 au. The dynamic NLO response of doped LiBHHTP complexes is also high, where the values are ranged in between 3.67×10^5 and 6.04×10^8 au at 1064 nm. This article not only highlights the effects of alkali atom doping on the NLO behavior of materials but

also presents the first Lithiated boron-containing triphenylene as a next-generation optoelectronic material.

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6. Allangawi, A., Sajid, H., Ayub, K., Gilani, M. A., Akhter, M. S., & Mahmood, T. (2023). High drug carrying efficiency of boron-doped Triazine based covalent organic framework toward anti-cancer tegafur; a theoretical perspective. Computational and Theoretical Chemistry, 1220, 113990.

ABSTRACT:
The therapeutic potential of Triazines-based six-membered ring covalent organic framework (COF) and respective boron doped derivative toward anticancer drug *i.e.*, Tegafur (TG) is evaluated using the first principles DFT calculations. The geometric, energetic, and electronic properties of TG@Triazine and TG@TriazineB2 are computed to explore and compare the efficacy of selected COFs as drug carrier systems. The strength of the adsorption of tegafur onto the triazine-COFs is illustrated through the counterpoise corrected adsorption energies (*Ecp*). The computed *Ecp* of TG@Triazine and TG@TriazineB2 are −21.81 and −25.57 kcal/mol, which illustrate the physisorption of the drug on adsorbent. The nature of interactions *i.e.*, physisorption between tegafur and Triazine COFs is further illustrated *via* the noncovalent interaction index (NCI) plot and quantum theory of atom in molecules (QTAIM), which illustrated that the weak dispersion forces are present between the drug and COF adsorbents. In comparison, the adsorption strength is significantly high in boronated triazineB2 COF. The electronic properties, including HOMO-LUMO analysis and NBO charge transfer analysis, reveal the significant variation in the electronic behavior of triazine COF, upon doping with boron, the E_g (HOMO-LUMO gap) of pristine Triazine (4.15 eV) reduced to 0.49 eV in TriazineB2 analogue. This significant decrease in the E_g of Triazine on boron doping illustrates the shifting of the semiconducting behavior of pristine Triazine to the metallic nature of TriazineB2, thus the electron transportation becomes double the magnitude (0.018 |e|) on interaction with tegafur drug as compared to 0.07 |e| in TG@Triazine. Finally, the recovery time is computed to illustrate the time taken by the drug in detaching at the active site. With this study, it is confirmed that the triazine-COF can be a significant drug carrier, however, the doping of boron further enhances the therapeutic potential of the adsorbent.

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7. Khalid, M. T., Anjum, T., Khan, A. L., Rehman, F., Aslam, M., Gilani, M. A., ... & Yasin, M. (2023). Task-specific polymeric membranes to achieve high gas-liquid mass transfer. Chemosphere, 313, 137603.

ABSTRACT:
In the current study, Polyimide (P84)-based polymeric membranes were fabricated and used as spargers in the bubble column reactor (BCR) to get a high gas-liquid mass transfer (GL-MT) rate of oxygen in water. Different polymeric membranes were fabricated by

incorporating polyvinyl pyrrolidone (PVP) as a porogen and a Zeolitic Imidazolate Framework (ZIF-8) to induce high porosity and hydrophobicity in the membranes. The GL-MT efficiency of membranes was evaluated by measuring the overall volumetric mass transfer coefficient (k_La) of oxygen in air. The k_La of O_2 (in air) was measured by supplying the gas through a fixed membrane surface area of 11.94 cm^2 at a fixed gas flow rate of 3L/min under atmospheric pressure. The results revealed that adding porogen and ZIF-8 increased the porosity of the membranes compared to the pure polymeric membranes. In comparison, the ZIF-8 (3 wt%) based membrane showed the highest porosity (80%), hydrophobicity (95° contact angle) and k_La of oxygen in air (241.2 h^{-1}) with 78% saturation in only 60 s. ZIF-8 based membranes showed the potential to increase the amount of dissolved oxygen in BCR by reducing the bubble size, increasing the number of bubbles, and improving the hydrophobicity. The study showed that ZIF-8 based membrane diffusers are expected to produce high GL-MT in microbial syngas fermentation. To the best of our knowledge, this is the first study on the fabrication and application of polymeric membranes for GL-MT applications. Further research should be conducted under real fermentation conditions to assess the practicality of the system to support substrate utilization, microbial growth, and product formation.

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8. Rehman, F., Khan, A. J., Alobaid, H. M., Gilani, M. A., Safi, S. Z., Muhammad, N., ... & Emran, T. B. (2023). Surface engineered mesoporous silica carriers for the controlled delivery of anticancer drug 5-fluorouracil: Computational approach for the drug-carrier interactions using density functional theory. Frontiers in Pharmacology, 14, 1146562.

ABSTRACT:

Introduction: Drug delivery systems are the topmost priority to increase drug safety and efficacy. In this study, hybrid porous silicates SBA-15 and its derivatives SBA@N and SBA@3N were synthesized and loaded with an anticancer drug, 5-fluorouracil. The drug release was studied in a simulated physiological environment.

Method: These materials were characterized for their textural and physio-chemical properties by scanning electron microscopy (SEM), nuclear magnetic resonance (NMR), Fourier transform infrared spectroscopy (FTIR), small-angle X-ray diffraction (SAX), and nitrogen adsorption/desorption techniques. The surface electrostatics of the materials was measured by zeta potential.

Results: The drug loading efficiency of the prepared hybrid materials was about 10%. *In vitro* drug release profiles were obtained in simulated fluids. Slow drug release kinetics was observed for SBA@3N, which released 7.5% of the entrapped drug in simulated intestinal fluid (SIF, pH 7.2) and 33% in simulated body fluid (SBF, pH 7.2) for 72 h. The material SBA@N presented an initial burst release of 13% in simulated intestinal fluid and 32.6% in simulated gastric fluid (SGF, pH 1.2), while about 70% of the drug was released within the next 72 h. Density functional theory (DFT) calculations have also supported the slow drug release from the SBA@3N material. The release mechanism of the drug from the prepared carriers was studied by first-order, second-order, Korsmeyer–Peppas, Hixson–Crowell, and Higuchi kinetic models. The

drug release from these carriers follows Fickian diffusion and zero-order kinetics in SGF and SBF, whereas first-order, non-Fickian diffusion, and case-II transport were observed in SIF.
Discussion: Based on these findings, the proposed synthesized hybrid materials may be suggested as a potential drug delivery system for anti-cancer drugs such as 5-fluorouracil.

Web URL:
https://www.frontiersin.org/journals/pharmacology/articles/10.3389/fphar.2023.1146562/full

9. Tayyab, M., Khan, M. I., Ahmad, A., Gilani, M. A., & Rahim, A. (2023). Development and characterization of nano-MOFs. In Nanomaterial-Based Metal Organic Frameworks for Single Atom Catalysis (pp. 107-138). Elsevier.

ABSTRACT:
In the modern era, metal–organic frameworks (MOFs) have gained more importance compared to conventional single-atom catalysts. MOFs have been synthesized with different methods like solvothermal, ion-thermal, microwave, mechanochemical, sonochemical, and electrochemical and have very specific porous structures, fine ultrahigh surface areas, selectivity, fine designability, and hollow and core structures. Because of these properties, MOF materials are used in different applications like water remediation treatment, heavy metal separation, volatile organic compound degradation, catalytic degradation, and specific target sensing. Nanomaterial-based MOF structures are used in a very wide application spectrum, and their importance and applications are discussed.

Web URL: https://www.sciencedirect.com/science/article/abs/pii/B9780128245248000025

10. Allangawi, A., Mahmood, T., Ayub, K., & Gilani, M. A. (2023). Anchoring the late first row transition metals with B12P12 nanocage to act as single atom catalysts toward oxygen evolution reaction (OER). Materials Science in Semiconductor Processing, 153, 107164.

ABSTRACT:
The high over-potential associated with water splitting hinders the wide production of hydrogen and oxygen gases. Recent advancements in this field are being made by exploring novel, low-cost and highly efficient catalysts to lower the over-potential of the water splitting reaction. Herein, we studied the novel single atom catalysts (SACs) based on late first-row transition metal doped boron phosphide ($B_{12}P_{12}$) nano-cages for the electrocatalysis of the oxygen evolution reaction (OER) via density functional theory (DFT) calculations. The choice of using boron phosphide nano-cages as the support is based on the highly desirable properties within it. Namely, having many defects, excellent electrical conductivity, large surface area, and high chemical stability. The Ni@$B_{12}P_{12}$ and Co@$B_{12}P_{12}$ SACs exhibit high chemical stability, having interaction energies of −1.70 and −2.55 eV, respectively. Moreover, the results of quantum theory of atoms in molecules (QTAIM) analysis confirmed that the transition metals are covalently chemisorbed on the nano-cages, such strong interactions are desirable in SACs to ensure they withstand harsh chemical environments and are active for longer time period. Frontier molecular orbitals (FMOs) analysis indicates that the designed catalysts have semi-

conducting capabilities which facilitate the transfer of electrons. The calculated FMOs energy gap (H-L E_{gap}) values range from 2.01 to 2.88 eV. Results of OER activity analysis indicate that Ni@$B_{12}P_{12}$ and Co@$B_{12}P_{12}$ are promising OER SACs with low overpotentials (1.01 and 1.06 V, respectively). The result of this study highlights the viability of $B_{12}P_{12}$ nano-cages as supports in SACs and encourage the exploration of other nano-cages in the catalysis field.

Web URL: https://www.sciencedirect.com/science/article/pii/S1369800122006904

11. Akhter, P., Bhatti, T. Y., Shafiq, I., Jamil, F., Nazar, R., Nazir, M. S., ... & Park, Y. (2023). Antioxidant activity of sea buckthorn (Hippophae rhamnoides) seed oil extracted using various organic solvents. Korean Journal of Chemical Engineering, 40(12), 2914-2920.

ABSTRACT:

Sea buckthorn (SBT) combines very fascinating nutritional composition with vital vitamins (A, C, E, D, K, and B complexes). Flavonoids, sterols, *α*-carotene, linoleic acid, and many more unsaturated fatty acids are present in the sea buckthorn plant. The organic extract of SBT seeds is commonly utilized as an anti-aging ingredient in numerous cosmetics. SBT oil extracts are used in pharmaceuticals that treat diseases like diabetes, cancer, cardiovascular disease, and neurological disorders, in addition to cosmetology. In this investigation, various concentrations of organic solvents such as *n*-hexane, isopropyl alcohol, ethyl acetate, ethanol, methanol, and ascorbic acid (standard) were used for the extraction of oil from sea buckthorn seeds. The antioxidant activity of such extracts was checked by the iron chelating, commonly known as the ferric chloride ($FeCl_3$) method, which is based on the ferric reducing ability of plasma (FRAP) assay with the help of UV-Vis. Our results indicate that seed extract of *Hippophae rhamnoides*, should be considered as a non-toxic source and the ferric reducing ability of plasma (FRAP) assay is used to evaluate the anti-oxidant potential by various organic solvents. The highest (68%) of FRAP is scavenged by the ethyl acetate and least (53%) of isopropyl extracts.

Web URL: https://link.springer.com/article/10.1007/s11814-023-1453-8

12. Akhter, P., Bhatti, T. Y., Shafiq, I., Jamil, F., Nazar, R., Nazir, M. S., ... & Park, Y. (2023). Antioxidant activity of sea buckthorn (Hippophae rhamnoides) seed oil extracted using various organic solvents. Korean Journal of Chemical Engineering, 40(12), 2914-2920.

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Sea buckthorn (SBT) combines very fascinating nutritional composition with vital vitamins (A, C, E, D, K, and B complexes). Flavonoids, sterols, *α*-carotene, linoleic acid, and many more unsaturated fatty acids are present in the sea buckthorn plant. The organic extract of SBT seeds is commonly utilized as an anti-aging ingredient in numerous cosmetics. SBT oil extracts are used in pharmaceuticals that treat diseases like diabetes, cancer, cardiovascular disease, and neurological disorders, in addition to cosmetology. In this investigation, various concentrations of organic solvents such as *n*-hexane, isopropyl alcohol, ethyl acetate, ethanol, methanol, and

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Web URL: **https://link.springer.com/article/10.1007/s11814-023-1453-8**

13. Iqbal, M. A., Akhter, T., Faheem, M., Mahmood, A., Al-Masry, W., Nadeem, S., ... & Park, C. H. (2023). Metal-free, visible light-mediated atom transfer radical polymerization of hydroxypropyl cellulose-graft-poly (methyl methacrylate) s: effect of polymer side chains on thermo-responsive behavior of hydroxypropyl cellulose. Cellulose, 30(12), 7519-7533.

ABSTRACT:
We exploited organic photo-redox-catalyzed atom transfer radical polymerization (O-ATRP) to synthesize a thermo-responsive polymer with a narrow molecular weight distribution. Poly(methyl methacrylate) (PMMA) chains were polymerized from a hydroxypropyl cellulose (HPC)-based macroinitiator using metal-free O-ATRP under visible-light irradiation. This O-ATRP is mediated by 1,2,3,5-tetrakis (carbazol-9-yl)-4,6-dicyanobenzene (4CzIPN), a photoredox catalyst with a substantial excited-state reduction potential, low cost, and ease of preparation. The synthesis of a series of PMMA-grafted HPC (PMMA-*g*-HPC) was characterized by various analytical methods, including FTIR spectroscopy, NMR spectroscopy, TGA, and GPC analysis. The lower critical solution temperature (LCST) of the polymers was determined by measuring the transmittance of the polymer solution as a function of the temperature at various pH values. Consequently, we expanded the LCST window of the HPC-based polymers and generated the opposite pH dependency of the LCST by forming PMMA-*g*-HPCs. Our "grafting-from" synthetic approach and thermo-responsive polymers, which are controllable in full range of physiological conditions, are promising in a variety of biological, electronics, and biosensor applications, particularly in drug delivery systems.

Web URL: https://link.springer.com/article/10.1007/s10570-023-05345-y

14. Siddiqa, A., Akhter, T., Faheem, M., Razzaque, S., Mahmood, A., Al-Masry, W., ... & Park, C. H. (2023). Bismuth-rich Co/Ni bimetallic metal–organic frameworks as photocatalysts toward efficient removal of organic contaminants under environmental conditions. Micromachines, 14(5), 899.

ABSTRACT:
Active photocatalysts with an efficiency of 99% were prepared for the degradation of the industrial dye, methylene blue (MB), under visible light irradiation. These photocatalysts comprised Co/Ni-metal–organic frameworks (MOFs), to which bismuth oxyiodide (BiOI) was added as a filler to prepare Co/Ni-MOF@BiOI composites. The composites exhibited

remarkable photocatalytic degradation of MB in aqueous solutions. The effects of various parameters, including the pH, reaction time, catalyst dose, and MB concentration, on the photocatalytic activity of the prepared catalysts were also evaluated. We believe that these composites are promising photocatalysts for the removal of MB from aqueous solutions under visible light.

Web URL: https://www.mdpi.com/2072-666X/14/5/899

15. Hassan, A. U., Mohyuddin, A., Güleryüz, C., Nadeem, S., Nkungli, N. K., Hassan, S. U., & Javed, M. (2023). Novel pull–push organic switches with D–π–A structural designs: computational design of star shape organic materials. Structural Chemistry, 34(2), 399-412.

ABSTRACT:

The structural alteration with π-linkers was used to design a donor–acceptor type series of 2,2′-(pyrimidine-4,6-diyl)bis(2,3-dihydro-1,3-benzothiazole) (**PB**)-based chromophores (**AH1**–**AH7**) to exploit the adjustments in their optical characteristics. To investigate the electronic geometries, absorption wavelengths, charge transfer processes, and the effect of structural alterations on nonlinear optical (NLO) characteristics, density functional theory (DFT) simulations have been used. During the UV–visible study, several long-range and range separated functionals like B3LYP, CAM-B3LYP, B97XD, and APFD with the 6-311G + (d,p) basis set were used to select the efficient level at DFT. As a response, UV–vis data indicated an intriguing consistency at the B3LYP level across experimental and TD-DFT-based values of **PB**. All the designed molecules had a smaller energy band gap (0.84–3.67 eV) and wide absorption spectra inside the visible region. Natural bond orbital (NBO) results indicated a significant push–pull operation, with donors and π-conjugates exhibiting positive values and most acceptors exhibiting the minimum values. Electronic transformations between electron donors to acceptor moiety, Trifluoromethyl (**TFM**) via π-conjugated linkers were shown to have a superior linear $<\alpha>$ and nonlinear (β_{total}) NLO values of 306–474 and 40–230 Debye-Angstrom^{-1} respectively. When chromophores with one phenyl π-linker were compared to those with the two π-linkers, the chromophores with the higher π-linker showed increased hyperpolarizability. The highest second-order hyperpolarizability (β) was found to be 230.11 Debye-Angstrom^{-1} which was about five times higher than urea (standard). This research has shown that by manipulating the kind of π-spacers, novel metal-free NLO compounds may be created, which might be used for high-tech NLO purposes.

Web URL: https://link.springer.com/article/10.1007/s11224-022-01983-3

16. Hassan, S. U., Shafique, S., Palvasha, B. A., Saeed, M. H., Naqvi, S. A. R., Nadeem, S., ... & Park, Y. K. (2023). Photocatalytic degradation of industrial dye using hybrid filler impregnated poly-sulfone membrane and optimizing the catalytic performance using Box-Behnken design. Chemosphere, 313, 137418.

ABSTRACT:

Mixed Matrix Membranes have gained significant attention over the past few years due to their diverse applications, unique hybrid inorganic filler and polymeric properties. In this article, the impregnation of nano-hybrid filler (polyoxometalates (~POMs) encapsulated into the metal-organic framework (MOF) ~ PMOF) on the polysulfone membrane (~PSF) was done, resulting in a mix matrix membrane (~PMOF@PSF). The developed structure was characterized by Fourier transform infrared (FT-IR), powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and transmission electron microscopes (TEM). The results confirmed that the nano-hybrid filler was successfully fabricated on the surface of PSF. Different loading ratios of nano-hybrid filler (5%, 10%, 20%, 30%, and 40%) were used for impregnation. The study's objective was to enhance catalytic performance using optimization curves designed using a three-level Box-Behnken Design (BBD) simulation. The photodegradation of Methylene Blue (~MB) was studied against PMOF@$PSF_{30\%}$ and was found to perform optimally when the concentration of catalyst, time of degradation, and temperature were 0.05–0.15 gm, 40–120 min, and 30–70 °C respectively. These experiments were replicated 15 times, and obtained results were further processed using a two-quadratic polynomial model to develop response surface methodology (RSM), which allowed for a functional relationship between the decolorization and experimental parameters. The optimal performance of the reaction mixture was calculated to be 0.15 gm for concentration, 70 °C for temperature, with an 80 min reaction time. Under these optimal conditions, the predicted decolorization of MB was 98.09%. Regression analysis with $R^2 > 0.99$ verified the fit of experimental results with predicted values. The PMOF@PSF $PSF_{30\%}$ demonstrated excellent reusability as its dye degradation properties were significantly unaffected after ten cycles.

Web URL: https://www.sciencedirect.com/science/article/pii/S004565352203911X

17. Ulfat, W., Mohyuddin, A., Amjad, M., Kurniawan, T. A., Mujahid, B., Nadeem, S., ... & Arif, M. (2023). Reuse of Buffing Dust-Laden Tanning Waste Hybridized with Poly-Styrene for Fabrication of Thermal Insulation Materials. Sustainability, 15(3), 1958.

ABSTRACT:

Air pollution, resulting from buffing dust waste produced by local leather tanning industry, has become a critical issue for the environment and public health. To promote a circular economy through resource recovery, this work developed a thermal insulation composite using buffing dust-laden tanning waste mixed with polystyrene and a blowing agent. To prepare the samples from leather tanning waste, different proportions of buffing dust (5–20% (*w*/*w*)) were blended with polystyrene in the presence of 3% (*w*/*w*) blowing agent. The composite material was processed in double-barreled with co-twin extruder to expose it to pressure and then heated at 200 °C. Different physico-chemical properties of composite samples were determined. The prepared composite materials had a good thermal conductivity (0.033–0.029 W/m-K), strong compression (5.21–6.25 ton), density (38–20 kg/m^3), and water absorption (5–7.5%), as compared to conventional constructional insulation panels. The thermal conductivity of polystyrene was reduced to 10% after the addition of buffing dust (20% *w*/*w*). The presence of a blowing agent in the composite material enhanced its volume without compromising its physico-chemical properties. Thermo-gravimetric analysis showed that the thermal stability of the composite material ranged from 200–412 °C. FTIR analysis indicated that the composite had

carbonyl and amino functional groups. The SEM images revealed the formation of voids with a decreasing homogeneity of the composite after the addition of the buffing dust waste. The EDX analysis revealed that the composite also had 62% of C and a tiny amount of Cr. This implies that the composite panels can be used for installation in buildings as thermal insulators in the construction sector. Overall, this work not only resolved the energy consumption problems during manufacturing, but it also brought positive impacts on the environment by recycling hazardous buffing dust and then reusing it as a thermal insulation material. Not only does this reduce the air pollution that results from the buffing dust waste, but this also promotes resource recovery in the framework of a circular economy.

Web URL: https://www.mdpi.com/2071-1050/15/3/1958

18. Aslam, A. A., Irshad, A., Nazir, M. S., & Atif, M. (2023). A review on covalent organic frameworks as adsorbents for organic pollutants. Journal of Cleaner Production, 400, 136737.

ABSTRACT:

Covalent organic frameworks (COFs) have attained substantial attention as promising candidate for pollutant adsorption due to extraordinary behavior in tunable porosity, large surface area, high crystallinity, reusability and surface chemistry. The data in this review has been compiled regarding mechanistic approaches of COFs towards adsorption of a variety of organic pollutants, including pharmaceutical, pesticides, dyes, and industrial waste. In addition, adsorption performance comparison has also been made between COFs and other materials. This review has latest data on the topic to understand and resolve present as well as future challenges.

Web URL: https://www.sciencedirect.com/science/article/pii/S0959652623008958

19. Mahboob, I., Shafiq, I., Shafique, S., Akhter, P., Munir, M., Saeed, M., ... & Hussain, M. (2023). Porous Ag3VO4/KIT-6 composite: Synthesis, characterization and enhanced photocatalytic performance for degradation of Congo Red. Chemosphere, 311, 137180.

ABSTRACT:

Novel Ag_3VO_4/KIT-6 nanocomposite photocatalyst has been successfully fabricated by a newly-designed simple hard-template induction process, in which the particles of Ag_3VO_4 were grown on the KIT-6 surface and inside the porous framework of the silica matrix. The developed porous framework nanocomposite was characterized by several techniques including N_2-Physiosorption analysis. The obtained nanocomposite revealed a high surface area (273.86 m^2/g) along with the possession of monoclinic Ag_3VO_4, which is highly responsive to visible light (with distinct intensity at about 700 nm). The UV–Vis DRS reveals that the Ag_3VO_4/KIT-6 photocatalyst bears a bandgap of 2.29 eV which confirms that the material has a good visible light response. The synthesized nanocomposite was tested for its superior physicochemical properties by evaluating its degradation efficiency for Congo Red (CR). The novel composite exhibited superior degradation capability of CR, reaching up to 96.49%, which was around three times the pure Ag_3VO_4. The detailed kinetic study revealed that the as-prepared material followed a pseudo first

order kinetic model for the CR degradation. The study includes a comprehensive parametric study for the formulation of the optimized reaction conditions for photocatalytic reactions. The commercial applicability of the composite material was investigated by a regeneration and recyclability test, which revealed extraordinary results. Furthermore, the possible degradation pathway for CR was also proposed.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653522036736

20. Ashraf, R., Sarfraz, A., Taskin-Tok, T., Iqbal, M. J., Iqbal, M. A., Iqbal, J., ... & Samir, A. (2023). Synthesis, molecular docking and anticancer potential of azolium based salts and their silver complexes: DNA/BSA interaction studies and cell cycle analysis. Journal of Molecular Liquids, 369, 120921.

ABSTRACT:
Azolium based molten salts have widely been investigated for biological potentials and interestingly, their metal complexes are getting attention in the field of medicinal inorganic chemistry. Here, we report three binuclear molten salts (**L1-L3**) and their silver complexes (**C1-C3**), assured through spectroscopic and mass spectrometric approaches. Solvent dependent catecholase activity was studied in three different solvents which suggests that nature of solvent has potential impact on chemical reactivity of test compounds. Anticancer activity was investigated through MTT assay, fluorescence microscopic analysis, ROS generation, and cell cycle arrest assay against HeLa, MCF-7, HCT-116 and A549 cancer cell lines and results confirmed the superior anticancer potential of silver complexes from their precursor salts. The cytotoxicity was cell selective and dose-dependant against MCF-7 with IC_{50} of C1 6.28 ± 0.82 μM which outshone even from positive control 5-FU (12.87 ± 1.0 μM) and cisplatin (8.74 ± 0.52 μM). Biological behavior of C1 & C2 was predicted through molecular docking studies and it speculated lower binding energies of C1 *i.e.* −10.05 kcal/mol and −7.51 kcal/mol for DNA and BSA, respectively. The experimental study of drug-DNA and drug-BSA interaction confirmed the prediction of simulation results. In addition, the role of hydrophobicity of compounds in the cytotoxicity was established viz., how the lipophilic value affects the anticancer activity of complexes.

Web URL: https://www.sciencedirect.com/science/article/pii/S0167732222024606

21. Ghafoor, M., Khan, Z. U., Nawaz, M. H., Akhtar, N., Rahim, A., & Riaz, S. (2023). In-situ synthesized ZIF-67 graphene oxide (ZIF-67/GO) nanocomposite for efficient individual and simultaneous detection of heavy metal ions. Environmental Monitoring and Assessment, 195(3), 423.

ABSTRACT:
Heavy metals are ubiquitous in water bodies as a result of anthropogenic activities and over time they accumulate in body thus posing serious health problems. Therefore, it is essential to improve sensing performance, for determination of heavy metal ions (HMIs), of electrochemical sensors. In this work, cobalt-derived MOF (ZIF-67) was in-situ synthesized and incorporated onto the surface of graphene oxide (GO) by simple sonication method. The prepared material

(ZIF-67/GO) was characterized by FTIR, XRD, SEM, and Raman spectroscopy. Afterwards, a sensing platform was made by drop-casting synthesized composite onto glassy carbon electrode for individual and simultaneous detection of heavy metal ions pollutants (Hg^{2+}, Zn^{2+}, Pb^{2+}, and Cr^{3+}) with estimated detection limits of 2 nM, 1 nM, 5 nM, and 0.6 nM, respectively, when determined simultaneously, that are below the permissible limit by World Health Organization. To the best of our knowledge, this is first report of HMIs detection by ZIF-67 incorporated GO sensor which can successfully determine the Hg^{+2}, Zn^{+2}, Pb^{+2}, and Cr^{+3} ions simultaneously with lower detection limits.

Web URL: https://link.springer.com/article/10.1007/s10661-023-10966-8

22. Batool, R., Riaz, S., Bano, S., Hayat, A., Nazir, M. S., Nasir, M., ... & Nawaz, M. H. (2023). Fabrication of polydopamine decorated carbon cloth as support material to anchor CeO2 nanoparticles for electrochemical detection of ethanol. Microchimica Acta, 190(5), 172.

ABSTRACT:

A flexible CeO_2 nanostructured polydopamine-modified carbon cloth (CeO_2/PDA/CC) interface was fabricated via electrodeposition for ethanol detection. The fabrication method involved two consecutive electrochemical steps in which dopamine was firstly electrodeposited on carbon fibers, followed by the electrochemical growth of CeO_2 nanoparticles. The CeO_2/PDA-based electroactive interface exerts an impressive electrochemical performance on the flexible sensor due to strong synergistic effect of the PDA functionalization with more active sites. Moreover, catalytic activity of CeO_2 nanostructures anchored on highly conductive CC incorporate superior electrocatalytic performance of the fabricated interface. The designed electrochemical sensor showed a wide response to ethanol in the linear range 1 to 25 mM with a detection limit of 0.22 mM. The CeO_2/PDA/CC flexible sensor showed good anti-interference ability and excellent repeatability and reproducibility (RSD = 1.67%). The fabricated interface performed well in saliva samples with satisfactory recoveries, corroborating the viability of CeO_2/PDA/CC integrated interface for practical implementation.

Web URL: https://link.springer.com/article/10.1007/s00604-023-05707-0

23. Shoukat, N., Anzar, S., Asad, M., Al-Sulami, A. I., Khalid, H., Choudhary, A. A., ... & Akhtar, N. (2023). Fabrication of CuO–NiO wrapped cellulose acetate/polyaniline electrospun nanofibers for sensitive monitoring of bisphenol-A. ACS Sustainable Chemistry & Engineering, 11(11), 4299-4307.

ABSTRACT:

Monitoring endocrine-disrupting chemicals such as bisphenol-A (BPA) is of great concern because its exposure may lead to reproductive problems, neurotoxicity, mutagenicity, and even carcinogenicity. Herein, we reported the fabrication of an efficient electrochemical sensor based on CuO–NiO wrapped cellulose acetate/polyaniline electrospun nanofibers at a Ni foam (CuO–NiO/CA–PANI@NF) electrode for the sensitive and selective monitoring of BPA. CA–PANI-

based electrospun nanofibers were selected because of their improved electrical conductivity and charge density, high binding affinity toward BPA via alternative amine and imine groups, and low cost, thus paving the way for the smooth and uniform flow of ions. However, CuO–NiO-based nanoparticles offer more exposed catalytic active species such as NiOOH/CuOOH for the fast electrocatalytic oxidation of BPA. Thus, the synergistic effect of CuO–NiO nanoparticles with electrospun nanofibers leads to high sensitivity (0.00172 μA/nM/cm^2) with a low limit of detection (0.6 nM), a wide linear range (2–100 nM), and high selectivity, even in the presence of interferences, including Co^{2+}, Cd^{2+}, Na^+ Pb^{2+}, Ni^{2+}, Cd^{2+}, Ca^{2+}, Fe^{3+}, NO_3^{2-}, SO_4^{2-}, Cr^{6+}, Br^-, Mg^{2+}, Zn^{2+}, and Ba^{2+} and molecules such as bisphenol-B, bisphenol-F, and phenol. The designed electrode was successfully applied to monitor BPA from plastic bottled water with high precision, thus suggesting the reliability of our designed system.

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https://pubs.acs.org/doi/full/10.1021/acssuschemeng.2c04482?casa_token=YJetBMyUPoAAAAAA%3A54YycZotW4e4O7FGlitHOFXii5NBawbNEu1V79m47CcwWgOT2nwjyPbOGjfPZaedfavZJYp_QYmcEd4

DEPARTMENT OF COMPUTER SCIENCES

1. Yasin, S., Othmani, A., Raza, I., & Hussain, S. A. (2023). Machine learning based approaches for clinical and non-clinical depression recognition and depression relapse prediction using audiovisual and EEG modalities: A comprehensive review. Computers in Biology and Medicine, 159, 106741.

ABSTRACT:
Mental disorders are rapidly increasing each year and have become a major challenge affecting the social and financial well-being of individuals. There is a need for phenotypic characterization of psychiatric disorders with biomarkers to provide a rich signature for Major Depressive Disorder, improving the understanding of the pathophysiological mechanisms underlying these mental disorders. This comprehensive review focuses on depression and relapse detection modalities such as self-questionnaires, audiovisuals, and EEG, highlighting noteworthy publications in the last ten years. The article concentrates on the literature that adopts machine learning by audiovisual and EEG signals. It also outlines preprocessing, feature extraction, and public datasets for depression detection. The review concludes with recommendations that will help improve the reliability of developed models and the determinism of computational intelligence-based systems in psychiatry. To the best of our knowledge, this survey is the first comprehensive review on depression and relapse prediction by self-questionnaires, audiovisual, and EEG-based approaches. The findings of this review will serve as a useful and structured starting point for researchers studying clinical and non-clinical depression recognition and relapse through machine learning-based approaches.

Web URL: https://www.sciencedirect.com/science/article/pii/S0010482523002068

2. Muneer, I., Saddique, M., Habib, Z., & Mohamed, H. G. (2023). Shoplifting Detection Using Hybrid Neural Network CNN-BiLSMT and Development of Benchmark Dataset. Applied Sciences, 13(14), 8341.

ABSTRACT:
Shoplifting poses a significant challenge for shop owners as well as other stakeholders, including law enforcement agencies. In recent years, the task of shoplifting detection has gained the interest of researchers due to video surveillance generating vast quantities of data that cannot be processed in real-time by human staff. In previous studies, different datasets and methods have

been developed for the task of shoplifting detection. However, there is a lack of a large benchmark dataset containing different behaviors of shoplifting and standard methods for the task of shoplifting detection. To overcome this limitation, in this study, a large benchmark dataset has been developed, having 900 instances with 450 cases of shoplifting and 450 of non-shoplifting with manual annotation based on five different ways of shoplifting. Moreover, a method for the detection of shoplifting is proposed for evaluating the developed dataset. The dataset is also evaluated with methods as baseline methods, including 2D CNN and 3D CNN. Our proposed method, which is a combination of Inception V3 and BILSTM, outperforms all baseline methods with 81 % accuracy. The developed dataset will be publicly available to foster in various areas related to human activity recognition. These areas encompass the development of systems for detecting behaviors such as robbery, identifying human movements, enhancing safety measures, and detecting instances of theft.

Web URL: https://www.mdpi.com/2076-3417/13/14/8341

3. Aslam, A., Sargano, A. B., & Habib, Z. (2023). Attention-based multimodal sentiment analysis and emotion recognition using deep neural networks. Applied Soft Computing, 144, 110494.

ABSTRACT:
There has been a growing interest in multimodal sentiment analysis and emotion recognition in recent years due to its wide range of practical applications. Multiple modalities allow for the integration of complementary information, improving the accuracy and precision of sentiment and emotion recognition tasks. However, working with multiple modalities presents several challenges, including handling data source heterogeneity, fusing information, aligning and synchronizing modalities, and designing effective feature extraction techniques that capture discriminative information from each modality. This paper introduces a novel framework called "Attention-based Multimodal Sentiment Analysis and Emotion Recognition (AMSAER)" to address these challenges. This framework leverages intra-modality discriminative features and inter-modality correlations in visual, audio, and textual modalities. It incorporates an attention mechanism to facilitate sentiment and emotion classification based on visual, textual, and acoustic inputs by emphasizing relevant aspects of the task. The proposed approach employs separate models for each modality to automatically extract discriminative semantic words, image regions, and audio features. A deep hierarchical model is then developed, incorporating intermediate fusion to learn hierarchical correlations between the modalities at bimodal and trimodal levels. Finally, the framework combines four distinct models through decision-level fusion to enable multimodal sentiment analysis and emotion recognition. The effectiveness of the proposed framework is demonstrated through extensive experiments conducted on the publicly available Interactive Emotional Dyadic Motion Capture (IEMOCAP) dataset. The results confirm a notable performance improvement compared to state-of-the-art methods, attaining 85% and 93% accuracy for sentiment analysis and emotion classification, respectively. Additionally, when considering class-wise accuracy, the results indicate that the "angry" emotion and "positive" sentiment are classified more effectively than the other emotions and sentiments, achieving 96.80% and 93.14% accuracy, respectively.

Web URL: https://www.sciencedirect.com/science/article/pii/S1568494623005124

4. Mumtaz, A., Sargano, A. B., & Habib, Z. (2023). Robust learning for real-world anomalies in surveillance videos. Multimedia Tools and Applications, 82(13), 20303-20322.

ABSTRACT:
Anomaly detection has significant importance for developing autonomous surveillance systems. Real-world anomalous events are far more complex and harder to capture due to diverse human behaviors and a wide range of anomaly types. A key factor in defining activity is the temporal length or duration of the activity. The time period required for an anomalous activity to be completely understandable and meaningful depends on the nature and speed of the event. Some events are as fast to be captured within a few frames; however, some activities are slow and may require several thousands of video frames to define an activity. Deep learning architectures have a limited input temporal sequence length and suffer from learning very long sequences. There is a need to re-investigate the problem from the frame sequences perspective to better define an activity in the limited temporal length. In this research work, our contribution is two-fold. Firstly, a novel strategy of dynamic frame-skipping is proposed for producing meaningful temporal sequences for model learning. Secondly, a new deep learning model based on the Inflated Inception network (I3D) is proposed for learning spatial and temporal information from video frames. In order to evaluate the performance of the proposed model, experiments are performed on one of the most challenging real-world anomalies UCF-Crime dataset. The results confirm that the proposed model is robust and significantly outperforms state-of-the-art methods in terms of accuracy. In addition to this, the proposed model has achieved the highest F1 score for fast and slow activities, such as explosions, road accidents, robbery, and stealing, and the AUC score of 0.837.

Web URL: https://link.springer.com/article/10.1007/s11042-023-14425-x

5. Farooque, G., Xiao, L., Sargano, A. B., Abid, F., & Hadi, F. (2023). A dual attention driven multiscale-multilevel feature fusion approach for hyperspectral image classification. International Journal of Remote Sensing, 44(4), 1151-1178.

ABSTRACT:
Deep learning has achieved promising results for hyperspectral image (HSI) classification in recent years due to its hierarchical structure and automatic feature extraction ability from raw data. The HSI has continuous spectral information, allowing for the precise identification of materials by capturing minute spectral differences. Convolutional neural networks (CNNs) have proven to be effective feature extractors for HSI classification. However, inherent network limitations prevent them from adequately mining and representing the sequence attributes of spectral signatures and learning critical and valuable features from both spectral and spatial dimensions simultaneously. This paper proposes a deep learning-based framework called a novel dual attention-based multiscale-multilevel ConvLSTM3D (DAMCL) to address these challenges. In this work, our contribution is threefold; firstly, a dual attention mechanism is proposed, effectively learning critical and valuable features from spectral and spatial dimensions. Secondly, multiscale ConvLSTM3D blocks can learn the discriminative features alongside handling long-

range dependencies of spectral data. Thirdly, these features are combined by a multilevel feature fusion approach to maximize the impact of features learned at different levels. To assess the performance of the proposed method, extensive experiments are carried out on five different benchmark datasets containing complex and challenging land cover classes. The results confirm that the proposed method outperforms state-of-the-art techniques with a small number of training samples in terms of overall accuracy (OA), average accuracy (AA), and Kappa (k)(�). The overall accuracy of 98.88%, 99.42%, 99.20%, 95.37%, and 92.57% is achieved over the Indian Pines, Salinas Valley, University of Pavia, Houston 2013, and Houston 2018 datasets, respectively.

Web URL: https://www.tandfonline.com/doi/full/10.1080/01431161.2023.2176721

6. Kaleem, M., Nazir, S., Jabeen, S., Mirza, H. T., Agha, S., & Raza, A. (2023). Sputtering Al2O3 enhanced bandgap engineering for integrated photonic devices. Optics & Laser Technology, 162, 109287.

ABSTRACT:
We present experimental results of the application of Sputtering enhanced Quantum Well Intermixing (QWI) process, where the bandgap of InGaAsP/InP quantum well laser microstructure is effectively modified by intermixing quantum well and potential barrier layers through sputtering Al_2O_3-QWI. This technique creates point defects through plasma induced disordering in the process of sputtering Al_2O_3. The subsequent Rapid thermal Anneal (RTA) process is performed to increase the diffusion rate and quantum well intermixing. This results in an increased transitional energy and hence it modifies the bandgap essential for the development of next generation complex photonic integrated circuits (ICs). We report a large bandgap blue shift of 144 nm is achievable with a very high increase in photoluminescence (PL) intensity. The experimental results of the bandgap shifted waveguides and laser diodes are presented. Photoluminescence (PL) measurements of InGaAsP/InP laser structure were taken before and after Al_2O_3-QWI process. The proposed technique can provide reliable and fast post-growth wafer level fabrication of photonic devices monolithically.

Web URL: https://www.sciencedirect.com/science/article/pii/S0030399223001809

7. Ahmad, M., Bajwa, U. I., Mehmood, Y., & Anwar, M. W. (2023). Lightweight ResGRU: a deep learning-based prediction of SARS-CoV-2 (COVID-19) and its severity classification using multimodal chest radiography images. Neural Computing and Applications, 35(13), 9637-9655.

ABSTRACT:
The new COVID-19 emerged in a town in China named Wuhan in December 2019, and since then, this deadly virus has infected 324 million people worldwide and caused 5.53 million deaths by January 2022. Because of the rapid spread of this pandemic, different countries are facing the problem of a shortage of resources, such as medical test kits and ventilators, as the number of cases increased uncontrollably. Therefore, developing a readily available, low-priced, and

automated approach for COVID-19 identification is the need of the hour. The proposed study uses chest radiography images (CRIs) such as X-rays and computed tomography (CTs) to detect chest infections, as these modalities contain important information about chest infections. This research introduces a novel hybrid deep learning model named *Lightweight ResGRU* that uses residual blocks and a bidirectional gated recurrent unit to diagnose non-COVID and COVID-19 infections using pre-processed CRIs. *Lightweight ResGRU* is used for multi-modal two-class classification (normal and COVID-19), three-class classification (normal, COVID-19, and viral pneumonia), four-class classification (normal, COVID-19, viral pneumonia, and bacterial pneumonia), and COVID-19 severity types' classification (i.e., atypical appearance, indeterminate appearance, typical appearance, and negative for pneumonia). The proposed architecture achieved f-measure of 99.0%, 98.4%, 91.0%, and 80.5% for two-class, three-class, four-class, and COVID-19 severity level classifications, respectively, on unseen data. A large dataset is created by combining and changing different publicly available datasets. The results prove that radiologists can adopt this method to screen chest infections where test kits are limited.

Web URL: https://link.springer.com/article/10.1007/s00521-023-08200-0

8. Zulfiqar, F., Bajwa, U. I., & Mehmood, Y. (2023). Multi-class classification of brain tumor types from MR images using EfficientNets. Biomedical Signal Processing and Control, 84, 104777.

ABSTRACT:
Accurate classification of the type of brain tumor plays an important role in the early diagnosis of the tumor which can be the difference between life and death. Magnetic Resonance Imaging (MRI) is commonly used to capture high-contrast grayscale images of the brain and is a non-invasive method for brain tumor diagnosis. Deep Learning (DL) using Convolutional Neural Networks (CNN) has revolutionized Computer Aided Diagnostic (CAD) systems by producing remarkable results for various medical imaging analysis tasks including brain tumor detection. In this research, a transfer learning-based fine-tuning approach for the classification of brain tumors into three classes i.e. glioma, meningioma, and pituitary tumor using EfficientNets is carried out. Five variants of pre-trained models from the EfficientNets family i.e. EfficientNetB0 – EfficientNetB4 are fine-tuned on publically available CE-MRI "Figshare – Brain Tumor Dataset". The proposed method of fine-tuning pre-trained EfficientNet is carried out by first loading ImageNet weights to the EfficientNet model followed by the addition of several top layers and a fully connected layer for the classification of brain tumor types. Several experiments are carried out to analyze the robustness of the proposed fine-tuned EfficientNets in comparison to other pre-trained models. Moreover, the effect of data augmentation on the model's test accuracy is also studied. Finally, the Grad-CAM visualization of the attention maps of the best model is presented that successfully highlights the tumorous region of the brain cell. The proposed method of fine-tuning pre-trained EfficientNet showed significant performance using EfficientNetB2 as a backbone achieving overall test accuracy, precision, recall/sensitivity, and F1-score of 98.86%, 98.65%, 98.77%, and 98.71% respectively. The proposed fine-tuned EfficientNetB2 is lightweight, computationally inexpensive (during training and inference), and

generalizes well. The source code is available at https://github.com/FatimaZulfiqar/multi-class-brain-tumor-classification

Web URL: https://www.sciencedirect.com/science/article/pii/S1746809423002100

9. Khan, H. R., Gillani, Z., Jamal, M. H., Athar, A., Chaudhry, M. T., Chao, H., ... & Chen, M. (2023). Early identification of crop type for smallholder farming systems using deep learning on time-series sentinel-2 imagery. Sensors, 23(4), 1779.

ABSTRACT:
Climate change and the COVID-19 pandemic have disrupted the food supply chain across the globe and adversely affected food security. Early estimation of staple crops can assist relevant government agencies to take timely actions for ensuring food security. Reliable crop type maps can play an essential role in monitoring crops, estimating yields, and maintaining smooth food supplies. However, these maps are not available for developing countries until crops have matured and are about to be harvested. The use of remote sensing for accurate crop-type mapping in the first few weeks of sowing remains challenging. Smallholder farming systems and diverse crop types further complicate the challenge. For this study, a ground-based survey is carried out to map fields by recording the coordinates and planted crops in respective fields. The time-series images of the mapped fields are acquired from the Sentinel-2 satellite. A deep learning-based long short-term memory network is used for the accurate mapping of crops at an early growth stage. Results show that staple crops, including rice, wheat, and sugarcane, are classified with 93.77% accuracy as early as the first four weeks of sowing. The proposed method can be applied on a large scale to effectively map crop types for smallholder farms at an early stage, allowing the authorities to plan a seamless availability of food.

Web URL: https://www.mdpi.com/1424-8220/23/4/1779

10. Mahmood, K., Rasool, G., Sabir, F., & Athar, A. (2023). An empirical study of web services topics in web developer discussions on stack overflow. IEEE Access, 11, 9627-9655.

ABSTRACT:
Web Services (WSs) are gaining worldwide popularity due to reliable and fast intercommunication services for the development of web and mobile applications. WSs are provided to client application developers through web Application Programming Interfaces (APIs), such as YouTube API, Twitter API, Facebook API, etc. Due to the popularity of WSs, the developers frequently discuss various WSs-based application' issues on online forums, such as Stack Overflow (SO). This study aims to highlight the problems faced by client developers in the development process of WSs-based applications using the dataset of SO. The comprehension of developers' conversations on SO can give insight into the frequency, difficulty, and popularity of different WSs-related problems of developers. We downloaded 12,746 posts from SO relevant to WSs-related issues for this article. We used the topic modeling technique (LDA) to extract various topics from the SO dataset. The topics are labeled and organized into categories and sub-categories according to relationships among them. The difficulty and popularity of each topic

have been analyzed. Our investigation yield several findings. First, developers focus on six topics related to WSs on SO: Client APIs development, Data Processing, Web services Authorization, Framework Support, Web APIs, and Mobile Applications. Secondly, the advantages and disadvantages of web applications topic (Fused_Popularity=0.39), from the Clients APIs development category have the highest prevalence, followed by Database (DB) and Data Processing in Applications topic (Fused_Popularity=0.38) from the Data Processing category. Third, most WSs-related topics in all categories are evolving promptly on SO, i.e., new questions are added daily about WSs development, deployment, and authorization. Fourth, the questions of type "how" are primarily asked in Framework support, Client APIs development, and Web APIs categories. Although, many questions in other categories are of the kin...

Web URL: https://ieeexplore.ieee.org/abstract/document/10024284

11. Altaf, A., Anwar, M. W., Jamal, M. H., & Bajwa, U. I. (2023). Exploiting linguistic features for effective sentence-level sentiment analysis in Urdu language. Multimedia Tools and Applications, 82(27), 41813-41839.

ABSTRACT:
Rapid increase in the use of social media has led to the generation of gigabytes of information shared by billions of users worldwide. To analyze this information and determine the behavior of people towards different events, sentiment analysis is widely used by researchers. Existing studies in Urdu sentiment analysis mostly use traditional n-gram features, which unlike linguistic features, do not focus on the contextual information being discussed. Moreover, no existing study classifies sentiments of proverbs and idioms which is challenging as mostly they do not contain sentiment words but carry strong sentiments. This study exploits linguistic features of Urdu language for sentence-level sentiment analysis and classifies idioms and proverbs using classical machine learning techniques. We develop a dataset comprising of idioms, proverbs, and sentences from the news domain, and extract part-of-speech tag-based features, boolean features, and numeric features from the dataset after keen linguistic analysis of Urdu language. Experimental results show that J48 classifier performs best in sentiment classification with an accuracy of 90% and an F-measure of 88%.

Web URL: https://link.springer.com/article/10.1007/s11042-023-15216-0

12. Hafeez, R., Anwar, M. W., Jamal, M. H., Fatima, T., Espinosa, J. C. M., López, L. A. D., ... & Ashraf, I. (2023). Contextual Urdu Lemmatization Using Recurrent Neural Network Models. Mathematics, 11(2), 435.

ABSTRACT:
In the field of natural language processing, machine translation is a colossally developing research area that helps humans communicate more effectively by bridging the linguistic gap. In machine translation, normalization and morphological analyses are the first and perhaps the most important modules for information retrieval (IR). To build a morphological analyzer, or to complete the normalization process, it is important to extract the correct root out of different

words. Stemming and lemmatization are techniques commonly used to find the correct root words in a language. However, a few studies on IR systems for the Urdu language have shown that lemmatization is more effective than stemming due to infixes found in Urdu words. This paper presents a lemmatization algorithm based on recurrent neural network models for the Urdu language. However, lemmatization techniques for resource-scarce languages such as Urdu are not very common. The proposed model is trained and tested on two datasets, namely, the Urdu Monolingual Corpus (UMC) and the Universal Dependencies Corpus of Urdu (UDU). The datasets are lemmatized with the help of recurrent neural network models. The Word2Vec model and edit trees are used to generate semantic and syntactic embedding. Bidirectional long short-term memory (BiLSTM), bidirectional gated recurrent unit (BiGRU), bidirectional gated recurrent neural network (BiGRNN), and attention-free encoder–decoder (AFED) models are trained under defined hyperparameters. Experimental results show that the attention-free encoder-decoder model achieves an accuracy, precision, recall, and F-score of 0.96, 0.95, 0.95, and 0.95, respectively, and outperforms existing models.

Web URL: https://www.mdpi.com/2227-7390/11/2/435

13. Sharjeel, M., Muneer, I., Nosheen, S., Nawab, R. M. A., & Rayson, P. (2023). Cross-lingual Text Reuse Detection at Document Level for English-Urdu Language Pair. ACM Transactions on Asian and Low-Resource Language Information Processing, 22(6), 1-22.

ABSTRACT:

In recent years, the problem of Cross-Lingual Text Reuse Detection (CLTRD) has gained the interest of the research community due to the availability of large digital repositories and automatic Machine Translation (MT) systems. These systems are readily available and openly accessible, which makes it easier to reuse text across languages but hard to detect. In previous studies, different corpora and methods have been developed for CLTRD at the sentence/passage level for the English-Urdu language pair. However, there is a lack of large standard corpora and methods for CLTRD for the English-Urdu language pair at the document level. To overcome this limitation, the significant contribution of this study is the development of a large benchmark cross-lingual (English-Urdu) text reuse corpus, called the TREU (Text Reuse for English-Urdu) corpus. It contains English to Urdu real cases of text reuse at the document level. The corpus is manually labelled into three categories (Wholly Derived = 672, Partially Derived = 888, and Non Derived = 697) with the source text in English and the derived text in the Urdu language. Another contribution of this study is the evaluation of the TREU corpus using a diversified range of methods to show its usefulness and how it can be utilized in the development of automatic methods for measuring cross-lingual (English-Urdu) text reuse at the document level. The best evaluation results, for both binary ($F_1 = 0.78$) and ternary ($F_1 = 0.66$) classification tasks, are obtained using a combination of all Translation plus Mono-lingual Analysis (T+MA) based methods. The TREU corpus is publicly available to promote CLTRD research in an under-resourced language, i.e., Urdu.

Web URL:
https://dl.acm.org/doi/full/10.1145/3592761?casa_token=RVULbL_nePwAAAAA%3AvsJS

qU5tDql61eNyFeS--ruPpwXf3cQV_kBBBgFSeq-Qk0VG6coc8b4ab7SX7nyuh7DzcebXNMw

14. Hafeez, H., Muneer, I., Sharjeel, M., Ashraf, M. A., & Adeel Nawab, R. M. (2023). Urdu short paraphrase detection at sentence level. ACM Transactions on Asian and Low-Resource Language Information Processing, 22(4), 1-20.

ABSTRACT:
Paraphrase detection systems uncover the relationship between two text fragments and classify them as paraphrased when they convey the same idea; otherwise non-paraphrased. Previously, the researchers have mainly focused on developing resources for the English language for paraphrase detection. There have been very few efforts for paraphrase detection in South Asian languages. However, no research has been conducted on sentence-level paraphrase detection in Urdu, a low-resourced language. It is mainly due to the unavailability of the corpora that focus on the sentence level. The available related studies on the Urdu language only focus on text reuse detection tasks at the passage and document levels. Therefore, this study aims to develop a large-scale manually annotated benchmark Urdu paraphrase detection corpus at the sentence level, based on real cases from journalism. The proposed Urdu Sentential Paraphrases (USP) corpus contains 4,900 sentences (2,941 paraphrased and 1,959 non-paraphrased), manually collected from the Urdu newspapers. Moreover, several techniques were proposed, developed, and compared as a secondary contribution, including Word Embedding (WE), Sentence Transformers (ST), and feature-fusion techniques. N-gram is treated as the baseline technique for our research. The experimental results indicate that our proposed feature-fusion technique is the most suitable for the Urdu paraphrase detection task. Furthermore, the performance increases when features of the proposed (ST) and baseline (N-gram) are combined for the classification task. In addition, The proposed techniques have also been applied to the UPPC corpus to check their performance at the document level. The best result we obtained using the feature fusion technique ($F_1 = 0.855$). Our corpus is available and free to download for research purposes.

Web URL: https://dl.acm.org/doi/full/10.1145/3586009?casa_token=S-047hvZEy4AAAAA%3AH9qg5FoLSjrF4RO4_J58yZD2dYA1t5m0mStrkJxugbVo3o0H0KgKga_fkEHd8w2qqD7MHFfNFrI

15. Shafi, J., Adeel Nawab, R. M., & Rayson, P. (2023). Semantic Tagging for the Urdu Language: Annotated Corpus and Multi-Target Classification Methods. ACM Transactions on Asian and Low-Resource Language Information Processing, 22(6), 1-32.

ABSTRACT:
Extracting and analysing meaning-related information from natural language data has attracted the attention of researchers in various fields, such as natural language processing, corpus linguistics, information retrieval, and data science. An important aspect of such automatic information extraction and analysis is the annotation of language data using semantic tagging tools. Different semantic tagging tools have been designed to carry out various levels of semantic analysis, for instance, named entity recognition and disambiguation, sentiment analysis, word

sense disambiguation, content analysis, and semantic role labelling. Common to all of these tasks, in the supervised setting, is the requirement for a manually semantically annotated corpus, which acts as a knowledge base from which to train and test potential word and phrase-level sense annotations. Many benchmark corpora have been developed for various semantic tagging tasks, but most are for English and other European languages. There is a dearth of semantically annotated corpora for the Urdu language, which is widely spoken and used around the world. To fill this gap, this study presents a large benchmark corpus and methods for the semantic tagging task for the Urdu language. The proposed corpus contains 8,000 tokens in the following domains or genres: news, social media, Wikipedia, and historical text (each domain having 2K tokens). The corpus has been manually annotated with 21 major semantic fields and 232 sub-fields with the USAS (UCREL Semantic Analysis System) semantic taxonomy which provides a comprehensive set of semantic fields for coarse-grained annotation. Each word in our proposed corpus has been annotated with at least one and up to nine semantic field tags to provide a detailed semantic analysis of the language data, which allowed us to treat the problem of semantic tagging as a supervised multi-target classification task. To demonstrate how our proposed corpus can be used for the development and evaluation of Urdu semantic tagging methods, we extracted local, topical and semantic features from the proposed corpus and applied seven different supervised multi-target classifiers to them. Results show an accuracy of 94% on our proposed corpus which is free and publicly available to download.

Web URL: https://dl.acm.org/doi/full/10.1145/3582496

16. Ashraf, M. A., Nawab, R. M. A., & Nie, F. (2023). Tran-Switch: A transfer learning approach for sentence level cross-genre author profiling on code-switched English–RomanUrdu Text. Information Processing & Management, 60(3), 103261.

ABSTRACT:

Cross-genre author profiling aims to build generalized models for predicting profile traits of authors that can be helpful across different text genres for computer forensics, marketing, and other applications. The cross-genre author profiling task becomes challenging when dealing with low-resourced languages due to the lack of availability of standard corpora and methods. The task becomes even more challenging when the data is code-switched, which is informal and unstructured. In previous studies, the problem of cross-genre author profiling has been mainly explored for mono-lingual texts in highly resourced languages (English, Spanish, etc.). However, it has not been thoroughly explored for the code-switched text which is widely used for communication over social media. To fulfill this gap, we propose a transfer learning-based solution for the cross-genre author profiling task on code-switched (English–RomanUrdu) text using three widely known genres, Facebook comments/posts, Tweets, and SMS messages. In this article, firstly, we experimented with the traditional machine learning, deep learning and pre-trained transfer learning models (MBERT, XLMRoBERTa, ULMFiT, and XLNET) for the same-genre and cross-genre gender identification task. We then propose a novel Trans-Switch approach that focuses on the code-switching nature of the text and trains on specialized language models. In addition, we developed three RomanUrdu to English translated corpora to study the impact of translation on author profiling tasks. The results show that the proposed Trans-Switch model outperforms the baseline deep learning and pre-trained transfer learning models for cross-

genre author profiling task on code-switched text. Further, the experimentation also shows that the translation of RomanUrdu text does not improve results.

Web URL: https://www.sciencedirect.com/science/article/pii/S0306457322003624

17. Junaid Anjum, M., Anees, T., Tariq, F., Shaheen, M., Amjad, S., Iftikhar, F., & Ahmad, F. (2023). Space-air-ground integrated network for disaster management: Systematic literature review.

ABSTRACT:
The occurrence of any kind of natural disaster will eventually lead to the loss of life and property. Countries where such disasters occur make every effort to monitor such disasters and aid as quickly as possible. However, in some cases, a rescue cannot be sent because no information is available to initiate any type of rescue operation. This is usually because common disaster management systems (DMS) use on board or ground networks to route information from the disaster scene to rescue headquarters (HQ), which in most cases cannot provide the information efficiently. One effective approach is to use satellites in conjunction with existing air-to-ground systems. This study provides a comprehensive and systematic overview of the complexities of the space-air-ground integrated network (SAGIN) in disaster management applications, including different architectures and protocols. The main rationale behind this review is to provide an extensive analysis of existing disaster management systems that are making use of SAGIN. This paper also presents the taxonomy for disaster management systems and challenges. Moreover, this research work also highlights open research issues and challenges for any type of disaster scenario. Our results indicate that several challenges are faced by disaster management systems such as hardware-based challenges, network-based characteristics and communication protocols related challenges, availability and accuracy of imagery data, and security and privacy issues.

Web URL: https://www.hindawi.com/journals/acisc/2023/6037882/

18. Imran, M., & Ahmad, A. (2023). Enhancing data quality to mine credible patterns. Journal of Information Science, 49(2), 544-564.

ABSTRACT:
The importance of big data is widely accepted in various fields. Organisations spend a lot of money to collect, process and mine the data to identify patterns. These patterns facilitate their future decision-making process to improve the organisational performance and profitability. However, among discovered patterns, there are some meaningless and misleading patterns which restrict the effectiveness of decision-making process. The presence of data discrepancies, noise and outliers also impacts the quality of discovered patterns and leads towards missing strategic goals and objectives. Quality inception of these discovered patterns is vital before utilising them in making predictions, decision-making process or strategic planning. Mining useful and credible patterns over social media is a challenging task. Often, people spread targeted content for character assassination or defamation of brands. Recently, some studies have evaluated the

credibility of information over social media based on users' surveys, experts' judgement and manually annotating Twitter tweets to predict credibility. Unfortunately, due to the large volume and exponential growth of data, these surveys and annotation-based information credibility techniques are not efficiently applicable. This article presents a data quality and credibility evaluation framework to determine the quality of individual data instances. This framework provides a way to discover useful and credible patterns using credibility indicators. Moreover, a new Twitter bot detection algorithm is proposed to classify tweets generated by Twitter bots and real users. The results of conducted experiments showed that the proposed model generates a positive impact on improving classification accuracy and quality of discovered patterns.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/01655515211013693

19. Farooq, M. S., Khalid, H., Arooj, A., Umer, T., Asghar, A. B., Rasheed, J., ... & Yahyaoui, A. (2023). A conceptual multi-layer framework for the detection of nighttime pedestrian in autonomous vehicles using deep reinforcement learning. Entropy, 25(1), 135.

ABSTRACT:
The major challenge faced by autonomous vehicles today is driving through busy roads without getting into an accident, especially with a pedestrian. To avoid collision with pedestrians, the vehicle requires the ability to communicate with a pedestrian to understand their actions. The most challenging task in research on computer vision is to detect pedestrian activities, especially at nighttime. The Advanced Driver-Assistance Systems (ADAS) has been developed for driving and parking support for vehicles to visualize sense, send and receive information from the environment but it lacks to detect nighttime pedestrian actions. This article proposes a framework based on Deep Reinforcement Learning (DRL) using Scale Invariant Faster Region-based Convolutional Neural Networks (SIFRCNN) technologies to efficiently detect pedestrian operations through which the vehicle, as agents train themselves from the environment and are forced to maximize the reward. The SIFRCNN has reduced the running time of detecting pedestrian operations from road images by incorporating Region Proposal Network (RPN) computation. Furthermore, we have used Reinforcement Learning (RL) for optimizing the Q-values and training itself to maximize the reward after getting the state from the SIFRCNN. In addition, the latest incarnation of SIFRCNN achieves near-real-time object detection from road images. The proposed SIFRCNN has been tested on KAIST, City Person, and Caltech datasets. The experimental results show an average improvement of 2.3% miss rate of pedestrian detection at nighttime compared to the other CNN-based pedestrian detectors.

Web URL: https://www.mdpi.com/1099-4300/25/1/135

20. Rasool, G., Hussain, Y., Umer, T., Rasheed, J., Yeo, S. F., & Sahin, F. (2023). Design Patterns for Mobile Games Based on Structural Similarity. Applied Sciences, 13(2), 1198.

ABSTRACT:
Software design patterns have a proven impact on the quality of software applications and the development process of an application. The success of design patterns in the software industry

has attracted mobile game developers and researchers to apply patterns in the context of mobile games. Researchers have already proposed different frameworks and design patterns, but they are not truly beneficial for game developers. The high-level taxonomies can be adjuvant while proposing useful design patterns. The existing taxonomies for mobile games do not consider different parts of a game that outline top-level structure. In this paper, we propose a new taxonomy that emphasizes the top-level structure for identifying new design patterns for mobile games. We propose five novel generic design patterns that might be applied to the development of mobile games and other software applications. The presented design patterns are, in a true sense, programming patterns that outline top-level generic classes and interfaces, and that could be the basis for the development of new games. We developed four demo games by using these patterns for the realization of taxonomy and design patterns.

Web URL: https://www.mdpi.com/2076-3417/13/2/1198

21. Arsalan, A., Burhan, M., Rehman, R. A., Umer, T., & Kim, B. S. (2023). E-DRAFT: An Efficient Data Retrieval and Forwarding Technique for Named Data Network Based Wireless Multimedia Sensor Networks. IEEE Access, 11, 15315-15328.

ABSTRACT:

Wireless Multimedia Sensor Network (WMSN) is a wirelessly connected sensor network featuring multimedia devices such as cameras and microphones that can retrieve video and audio streams, photographs, and scalar sensor data. Because of the low cost of cameras and microphones, in addition to significant advances in distributed signal processing and multimedia data coding approaches, WMSNs can offer multimedia content. Moreover, the most critical difficulty in the implementation of WMSN is to improve the efficiency and lifetime of the network. The Named-Data Network (NDN) technique is used in WMSNs to increase communication and transmission mechanisms efficiency. NDN is thought to be one of the most demanding Internet architectures in the future. Unlike host-centric techniques that focus on the location of the content, NDN focuses on providing the content. In this paper, we propose a novel accumulative Interest-based content-store architecture for NDN-based WMSNs to improve the efficiency of individual nodes as well as the overall network. Furthermore, the proposed solution also controls packet flooding. The proposed scheme is named “Efficient Data Retrieval and Forwarding (E-DRAFT)”. Moreover, the ndnSIM simulator is used to run comprehensive simulations. Compared to existing methodologies, the simulation results reveal that the proposed approach stops additional packet flooding and effectively stores and retrieves Data packets with enhanced processing efficiency.

Web URL: https://ieeexplore.ieee.org/abstract/document/10042299

22. Butt, H., Khosa, I., & Iftikhar, M. A. (2023). Feature transformation for efficient blood glucose prediction in type 1 diabetes mellitus patients. Diagnostics, 13(3), 340.

ABSTRACT:

Diabetes Mellitus, a metabolic disease, causes the body to lose control over blood glucose regulation. With recent advances in self-monitoring systems, a patient can access their personalized glycemic profile and may utilize it for efficient prediction of future blood glucose levels. An efficient diabetes management system demands the accurate estimation of blood glucose levels, which, apart from using an appropriate prediction algorithm, depends on discriminative data representation. In this research work, a transformation of event-based data into discriminative continuous features is proposed. Moreover, a multi-layered long short-term memory (LSTM)-based recurrent neural network is developed for the prediction of blood glucose levels in patients with type 1 diabetes. The proposed method is used to forecast the blood glucose level on a prediction horizon of 30 and 60 min. The results are evaluated for three patients using the Ohio T1DM dataset. The proposed scheme achieves the lowest RMSE score of 14.76 mg/dL and 25.48 mg/dL for prediction horizons of 30 min and 60 min, respectively. The suggested methodology can be utilized in closed-loop systems for precise insulin delivery to type 1 patients for better glycemic control.

Web URL: https://www.mdpi.com/2075-4418/13/3/340

23. Zaman, S. K. U., Mustafa, S., Abbasi, H., Maqsood, T., Rehman, F., Khan, M. A., ... & Elmannai, H. (2023). Cooperative content caching framework using cuckoo search optimization in vehicular edge networks. Applied Sciences, 13(2), 780.

ABSTRACT:

Vehicular edge networks (VENs) connect vehicles to share data and infotainment content collaboratively to improve network performance. Due to technological advancements, data growth is accelerating, making it difficult to always connect mobile devices and locations. For vehicle-to-vehicle (V2V) communication, vehicles are equipped with onboard units (OBU) and roadside units (RSU). Through back-haul, all user-uploaded data is cached in the cloud server's main database. Caching stores and delivers database data on demand. Pre-caching the data on the upcoming predicted server, closest to the user, before receiving the request will improve the system's performance. OBUs, RSUs, and base stations (BS) cache data in VENs to fulfill user requests rapidly. Pre-caching reduces data retrieval costs and times. Due to storage and computing expenses, complete data cannot be stored on a single device for vehicle caching. We reduce content delivery delays by using the cuckoo search optimization algorithm with cooperative content caching. Cooperation among end users in terms of data sharing with neighbors will positively affect delivery delays. The proposed model considers cooperative content caching based on popularity and accurate vehicle position prediction using K-means clustering. Performance is measured by caching cost, delivery cost, response time, and cache hit ratio. Regarding parameters, the new algorithm outperforms the alternative.

Web URL: https://www.mdpi.com/2076-3417/13/2/780

24. Zaman, S. K. U., Maqsood, T., Rehman, F., Mustafa, S., Khan, M. A., Gohar, N., ... & Elmannai, H. (2023). Content Caching in Mobile Edge Computing Based on User Location

and Preferences Using Cosine Similarity and Collaborative Filtering. Electronics, 12(2), 284.

ABSTRACT:
High-speed internet has boosted clients' traffic needs. Content caching on mobile edge computing (MEC) servers reduces traffic and latency. Caching with MEC faces difficulties such as user mobility, limited storage, varying user preferences, and rising video streaming needs. The current content caching techniques consider user mobility and content popularity to improve the experience. However, no present solution addresses user preferences and mobility, affecting caching decisions. We propose mobility- and user-preferences-aware caching for MEC. Using time series, the proposed system finds mobility patterns and groups nearby trajectories. Using cosine similarity and CF, we predict and cache user-requested content. CF predicts the popularity of grouped-based content to improve the cache hit ratio and reduce delay compared to baseline techniques.

Web URL: https://www.mdpi.com/2079-9292/12/2/284

25. Afandi, W., Bukhari, S. M. A. H., Khan, M. U., Maqsood, T., Fayyaz, M. A., Ansari, A. R., & Nawaz, R. (2023). Explainable YouTube video identification using sufficient input subsets. IEEE Access, 11, 33178-33188.

ABSTRACT:
Neural network models are black boxes in nature. The mechanics behind these black boxes are practically unexplainable. Having the insight into patterns identified by these algorithms can help unravel important properties of the subject in query. These artificial intelligence based algorithms are used in every domain for prediction. This research focuses on patterns formed in network traffic that can be leveraged to identify videos streaming over the network. The proposed work uses a sufficient input subset (SIS) model on two separate video identification techniques to understand and explain the patterns detected by the techniques. The first technique creates the fingerprints of videos on a period-based algorithm to handle variable bitrate inconsistencies. These fingerprints are passed to a convolutional Neural Network (CNN) for pattern recognition. The second technique is based on traffic pattern plot identification that creates a graph of packet size with respect to time for each stream before passing that to a CNN as an image. For model explainability, a sufficient input subset (SIS) model is used to identify features that are sufficient to reach the same prediction under a certain threshold of confidence by the model. The generated SIS of each input sample is clustered using DBSCAN, K-Means, and cosine-based Hierarchical clustering. The clustered SIS highlight the common patterns for each class. The SIS patterns learnt by each model of three individual videos are discussed. Furthermore, these patterns are used to investigate misclassification and provide a rationale behind it to justify the working of the classifier model.

Web URL: https://ieeexplore.ieee.org/abstract/document/10080939

26. Bilal, A., Mirza, H. T., & Hussain, I. (2023). Identifying significant textual features in titles of Google play store applications and their influence on user review rating. Knowledge and Information Systems, 65(3), 1159-1178.

ABSTRACT:
User review rating of mobile applications is a crucial factor related to downloads and it greatly impacts the customer's decisions to prefer the applications with the highest (most positive) ratings. Whereas, titles are among the first information displayed to users when they search for any particular application and a compelling title can be a leading cause for an application's success. Hence, developer companies fashion (optimize) their application titles strategically, in such a way, that they are highly eye-catching and descriptive about application functionalities in an attempt to lure users to download and positively rate their applications. However, traditional literature may lack the scientific approaches which investigate what (specific) kind of textual features in application titles actually have a positive (or negative) effect on the review rating. Therefore, aim of this research work is to perform two separate kinds of scientific analyses to determine the impacts of unconscious (aspects usually not observed by users) and conscious (keyterms which are observed by users) features of Google-play store application titles on the user review rating. At first, for the investigation of unconscious aspects various machine learning algorithms are employed and secondly, for the conscious features another keyterms analysis is carried out. Overall, according to the results, certain unconscious aspects can lead towards the elevated review ratings in both cases of Applications and Games. Albeit, conscious aspects tend to have a positive impact only on the review ratings of Games.

Web URL: https://link.springer.com/article/10.1007/s10115-022-01799-x

27. Khan, F. A., Ahmad, F., Khan, A. A., & Wechtaisong, C. (2023). Process Discovery and Refinement of an Enterprise Management System. Comput. Syst. Sci. Eng., 44(3), 2019-2032.

ABSTRACT:
The need for the analysis of modern businesses is rapidly increasing as the supporting enterprise systems generate more and more data. This data can be extremely valuable for executing organizations because the data allows constant monitoring, analyzing, and improving the underlying processes, which leads to the reduction of cost and the improvement of the quality. Process mining is a useful technique for analyzing enterprise systems by using an event log that contains behaviours. This research focuses on the process discovery and refinement using real-life event log data collected from a large multinational organization that deals with coatings and paints. By investigating and analyzing their order handling processes, this study aims at learning a model that gives insight inspection of the processes and performance analysis. Furthermore, the animation is also performed for the better inspection, diagnostics, and compliance-related questions to specify the system. The configuration of the system and the conformance checking for further enhancement is also addressed in this research. To achieve the objectives, this research uses process mining techniques, ie process discovery in the form of formal Petri nets models with the help of process maps, and process refinement through conformance checking and enhancement. Initially, the identified executed process is reconstructed by using the process

discovery techniques. Following the reconstruction, we perform a deep analysis for the underlying process to ensure the process improvement and redesigning. Finally, some recommendations are made to improve the enterprise management system processes.

Web URL: https://link.springer.com/article/10.1007/s10115-022-01799-x

28. Asif, R., Farooq-i-Azam, M., Chaudary, M. H., Husen, A., & Hassan, S. R. (2023). A distance vector hop-based secure and robust localization algorithm for wireless sensor networks. Electronics, 12(10), 2237.

ABSTRACT:
Location information of sensor nodes in a wireless sensor network is important. The sensor nodes are usually required to ascertain their positions so that the data collected by these nodes can be labeled with this information. On the other hand, certain attacks on wireless sensor networks lead to the incorrect estimation of sensor node positions. In such situations, when the location information is not correct, the data may be labeled with wrong location information that may subvert the desired operation of the wireless sensor network. In this work, we formulate and propose a distance vector hop-based algorithm to provide secure and robust localization in the presence of malicious sensor nodes that result in incorrect position estimation and jeopardize the wireless sensor network operation. The algorithm uses cryptography to ensure secure and robust operation in the presence of adversaries in the sensor network. As a result of the countermeasures, the attacks are neutralized and the sensor nodes are able to estimate their positions as desired. Our secure localization algorithm provides a defense against various types of security attacks, such as selective forwarding, wormhole, Sybil, tampering, and traffic replay, compared with other algorithms which provide security against only one or two types. Simulation experiments are performed to evaluate the performance of the proposed method, and the results indicate that our secure localization algorithm achieves the design objectives successfully. Performance of the proposed method is also compared with the performance of basic distance vector hop algorithm and two secure algorithms based on distance vector hop localization. The results reveal that our proposed secure localization algorithm outperforms the compared algorithms in the presence of multiple attacks by malicious nodes.

Web URL: https://www.mdpi.com/2079-9292/12/10/2237

DEPARTMENT OF ECONOMICS

1. Aslam, A., Mudassir, M., Ghouse, G., & Farooq, A. (2023). Introducing Modern Human Capital Model. Journal of the Knowledge Economy, 1-12.

ABSTRACT:
In neo-classical economic growth theory, literature is evident of the reformist role of human capital accumulation. Conversely, this relationship is empirically weak in many countries. To fulfill this gap, we estimate a dynamic model of modern human capital theory and use it to analyze the prospects for economic growth in selected Asian countries. The basic research question is to see if the modern human capital growth model provides more adequate consideration to rhetoric theory by studying the linkages among human capital, institutions, and trade openness? We propose that institutional quality, which is an important element in determining the effects of economic growth, increases along with human capital. We also find considerable elasticities in their interactions with economic growth. Results provide empirical evidence in favor of a substitutionary effect, rather than the existence of a complementary effect. This suggests that the size of the increase in institutions and human capital may differ to catalyze the growth process. The study in hand contributes to the literature in three aspects: (i) it provides a modern theoretical explanation of the rhetoric human capital model (well cited in the literature on economics); (ii) it empirically provides evidence for human capital accumulation that cannot be achieved without improvements in institutional quality, and this has been ignored in the previous literature on Asian countries; (ii) it suggests policy-makers that their focus must go through mentioned channels, as the growth effect may be operating through co-existence of human capital accumulation and institutional quality.

Web URL: https://link.springer.com/article/10.1007/s13132-023-01296-8

2. Malik, S., Abbas, A., Shabbir, M. S., & Ramos-Meza, C. S. (2023). Business cycle fluctuations, foreign direct investment, and real effective exchange rate nexus among asian countries. Journal of the Knowledge Economy, 1-14.

ABSTRACT:
Asian economies had faced high economic instability as compared to advanced economies due to unstable exchange rates, financial dependence on advanced economies, and macroeconomic imbalances. To overcome uncertainty, earlier studies considered output volatility in the research models, while in this study, business cycle fluctuations are estimated through GDP de-trended through the Hodrick-Prescott filter, where the cyclical component of GDP is used as representative of business cycle fluctuations. This study has attempted to investigate the

determinants of business cycle fluctuations among 20 Asian economies in the short run and long run through the panel ARDL model during 1990–2015. ARDL method is used as it is more suitable for cyclical component data series as compared to the standard co-integration method. Data was taken from world development indicators published by World Bank. The unit root tests showed that all the series were stationary with a mix of level and first difference, confirming the suitability of the panel ARDL technique. Panel regression analysis showed the positive and significant impact of external debt, foreign direct investment, imports, and real effective exchange rate while the negative and significant influence of exports and net domestic credit on business cycle fluctuations. Short-run analysis depicted a significant ECM value which confirmed short-run convergence toward the equilibrium.

Web URL: https://link.springer.com/article/10.1007/s13132-023-01316-7

3. Khan, M. I., Bashir, Z., & Amir, H. (2023). Lucrative Role of Financial Institutions on Willful Default-Financial Risk, and Fiscal Recovery: Evidence from Judgements of Apex Courts in Pakistan. Journal of Development and Social Sciences, 4(2), 683-691.

ABSTRACT:
The study theoretically supports financial institutions regarding financial risk which can criminally proceed against customers, expose willfully default-financial risk or not? The FIO, 2001 and judgments of Apex Courts have privileges i.e. fiscal recovery of suits under FIO, 2001, Code of Civil Procedure (1908-Act, V), Code of Criminal Procedure (1898-Act, V) and judgements of Apex Courts. These are the domains on Willful Default financial risk. Overall results explored that FIO, 2001, Order 37 of CPC and judgments of Apex Courts support to protect rights and interests of financial institutions through Banking Courts but initiation of criminal proceedings shall be through investigation agencies (FIA and NAB), appointed by Federal Government section 20 (7) of FIO, 2001 and action accordingly. The theoretical view has important implications for financial institutions that they may consider FIO, 2001 as a safer flight during criminal proceedings through investigation agencies against customers with respect to Willful Default (WD) financial risk, and fiscal recovery. Moreover, the regulators may decide to control the financial position of banks due to willful default financial risk.

Web URL: https://ojs.jdss.org.pk/journal/article/view/521

4. Amir, H., Bilal, K., & Khan, M. I. (2023). Efficacy of Investment in Educational Institutes and Human Capital for Sustainable Economic Growth in Pakistan. Annals of Human and Social Sciences, 4(2), 586-598.

ABSTRACT:
Efficacy of investment in educational institutes, and human capital have drastic role in economic upturn. However, at various levels human capital demonstrated regarding infrastructure of education that becomes a more relevant measure of human capital alternative to enrollment at school in different institutions. This study has taken four decades annual data to investigate the association between educational institutions and human capital on economic upswing. The data

starts from 1978 to 2018. The Cob Douglas production function is used to determine the efficacy of human capital, and upswing of the economy in Pakistan. The overall results reveal that there is a significant role of human capital (educational institutions) in economic growth in the long run. It is also observed that long-term development across countries has been propelled by productivity growth at a higher scale. Economic upswing accelerates the labor productivity, if necessary, actions should be part of Government investment. The decisions, and policies in educational institutes should be positive and proof of safe flight through human capital efficacy.

Web URL: https://ojs.ahss.org.pk/journal/article/view/271

5. Kumar, R., Amir-ud-Din, R., Ahmed, J., Asim, M., Rashid, F., Khan, S. A., ... & Pongpanich, S. (2023). Correlates of early initiation of breast feeding and prelacteal feeding: a cross-sectional study in Sindh province of Pakistan. BMJ open, 13(2), e069902.

ABSTRACT:

Objectives

The objective of this study was to determine the prevalence and correlates of early initiation of breast feeding and prelacteal feeding in highly disadvantaged districts in Pakistan.

Design

This cross-sectional study design.

Settings

This study was carried out in twelve districts of the Sindh province of Pakistan.

Participants

A total of 4800 mothers with children under 2 years, selected through a multistage random sampling method.

Data analysis

Bivariate association, survival analysis (Kaplan-Meier and Cox proportional hazard techniques), multivariate linear regression and the ordinary least square model were used.

Results

The results show that the prevalence of early initiation of breast feeding was 68% and prelacteal feeding was 32%. Adequate treatment, proper guidance at antenatal care visits, postpartum health check, normal birth with skilled birth attendants, institutional birth, skin-to-skin contact at birth and birth size were all associated with early breastfeeding initiation ($p<0.001$). The odds of early initiation of breast feeding after birth are higher if the respondents received proper guidance (OR 2.05; 95% CI 1.02 to 4.11) or made skin-to-skin contact (OR 10.65; 95% CI 6.82 to 16.65). Bivariate association between the prelacteal feeding and a set of correlates suggests that all variables under study were significantly associated with the outcome variable of interest at a 95% or higher significance level. The factors which significantly reduced the odds of prelacteal feeding were adequate treatment (OR 0.29; 95% CI 0.23 to 0.37) and postpartum health check (OR 0.65; 95% CI 0.53 to 0.80).

Conclusion

Sudy concludes that the correlates like adequate treatment of mothers during labour, postpartum health check-up, normal birth with skilled birth attendants, institutional births and skin-to-skin contact between mother and the baby determine the early initiation of breast feeding and

prelecteal feeding. Early initiation of breast feeding needs to be encouraged, and communities must be educated against the use of prelacteal feeding.

Web URL: https://bmjopen.bmj.com/content/13/2/e069902.abstract

6. Amir-ud-Din, R., Naz, L., & Ali, H. (2023). Relationship between asset ownership and women's empowerment? Evidence from DHS data from 18 developing countries. Journal of Demographic Economics, 1-22.

ABSTRACT:
This study identifies the link between women's asset ownership and women's empowerment. Women's empowerment is measured by their decision-making role related to their health, large household purchases, and their social interaction. Using Demographic and Health Surveys data for 18 countries from South Asia, the Middle East, and sub-Saharan Africa, we found that the women who owned assets were 14% more likely to be empowered compared with the women who did not own any asset (odds ratio: 1.14, 95% confidence interval: 1.10–1.185). At a disaggregated country level, asset ownership was positively and significantly associated with women's empowerment in nine countries, negatively associated in one country, and had no significant association in the other eight countries. This study provides important insights into the link between women's asset ownership and empowerment and may inform public policy related to gender equality through women's empowerment.

Web URL: https://www.cambridge.org/core/journals/journal-of-demographic-economics/article/abs/relationship-between-asset-ownership-and-womens-empowerment-evidence-from-dhs-data-from-18-developing-countries/58D70ECF4CD92E572280AA519D560C1B

7. Atif, R. M., Saqib, N., & Mahmood, H. (2023). Heterogeneity, sunk cost, and export performance: A firm level study of Pakistan's textile sector. Heliyon, 9(7).

ABSTRACT:
The textile sector is a significant exporting sector of Pakistan. This study examines the determinants of the export performance of Pakistani textile firms using firm-level panel data from 2008 to 2018. Under the framework of the dynamic System Generalized Method of Moment (SGMM) methodology, our findings suggest that both sunk costs and firm-specific characteristics like productivity, age, and size are important determinants of textile exports. Further, the study also observes that firms with a high number of export destinations and greater product diversification tend to export more. The year-specific dummies reveal that textile export performance is adversely affected by the energy crisis in 2012. We recommend that Pakistan should support large, experienced, and productive textile exporter firms to boost textile exports. Besides, more assistance should be provided regarding potential overseas markets to the existing and new export firms.

Web URL:
https://scholar.google.com/scholar?hl=en&as_sdt=0%2C5&q=+Heterogeneity%2C+sunk+cost+and+export+performance%3A+a+firm+level+study+of+Pakistan%E2%80%99s+textile+sector+&btnG=

DEPARTMENT OF ELETRICAL COMPUTER ENGINEENRING

1. Naseem, T., Javed, A., Hamayun, M. T., Jawad, M., Ansari, E. A., Fayyaz, M. A., ... & Nawaz, R. (2023). Design of an EnergyPlus model-based smart controller for maintaining thermal comfortable environment in non-domestic building. IEEE Access, 11, 33134-33147.

Abstract
Heating, Ventilation, and Air Conditioning (HVAC) systems account for 59% of energy consumption in domestic buildings and 36% in non-domestic buildings. According to a study, around 39% of occupants are dissatisfied with indoor temperature in non-domestic buildings. To maintain thermal comfort and indoor air quality, HVAC systems are widely used in non-domestic buildings. This research aims to develop energy-efficient control techniques for HVAC systems while ensuring indoor thermal comfort. Three control strategies, namely EnergyPlus model-based Model Predictive Control (MPC), Sliding Mode Control (SMC), and simple ON/OFF control, are employed and compared at the Department of Electrical and Computer Engineering, COMSATS University Islamabad, Lahore Campus. Furthermore, a machine learning-based Predicted Mean Vote (PMV)-based temperature setpoint estimator is designed to ensure occupant thermal comfort. The control techniques estimate the temperature setpoints and supply air temperature of the Variable Air Volume (VAV) system to control indoor room temperature. The energy consumption and indoor thermal comfort of the building are compared under different control techniques. The results show that MPC with PMV-based setpoints consumes 17.20% less energy during winters and 14.67% less energy during summers than a simple ON/OFF controller.

Web URL: https://ieeexplore.ieee.org/abstract/document/10086530

2. Akhtar, S., Nadeem, M., Rashdan, M., Hussain, B., Ansari, E. A., & Aslam, M. H. (2023). Online Mode of Teaching and Learning Process in Engineering Discipline: Teacher Perspective on Challenges Faced and Recommendations. Education Sciences, 13(2), 200.

Abstract
The COVID-19 pandemic has affected people from almost every walk of life in general and academia in particular. It had a huge impact on teaching and learning resulting in a sudden shift from classroom and face-to-face teaching to distance and online teaching and learning. This sudden shift created a lot of ruckuses in the teaching of engineering disciplines. This study is pertinent to the examination of faculty perceptions of online teaching in Pakistani universities and the obstacles they face in teaching engineering students through the online mode during this pandemic. The research takes a quantitative and sample survey approach. A Google form

questionnaire was used to collect the data from a sample of 91 faculty members from the engineering discipline of different universities in Pakistan during 2022. According to the study's findings, faculty generally have a favorable opinion of virtual teaching in the context of COVID-19 for closing the achievement gap and guiding students' futures in difficult times. However, they ran into a number of challenges when teaching online, including technological difficulties, problems with student participation, challenges with online tests and assessments, etc. The results of this study will urge educational institutions and policymakers to use the most up-to-date instructional methodologies and offer teachers ongoing professional development in order to improve the quality of online teaching, learning, and assessment in universities. Previous studies discussed a number of obstacles faced by students in virtual teaching in higher education, overlooking the perception and challenges faced by the engineering faculty. The present study replenishes this gap.

Web URL: https://www.mdpi.com/2227-7102/13/2/200

3. Iqbal, M. U., Ansari, E. A., Akhtar, S., Rafiq, M. N., Farooq-i-Azam, M., & Hassan, B. (2023). Hybrid Learning based Radio Resource Management in 5G Heterogeneous Networks. Pakistan Journal of Engineering and Technology, 6(1), 92-97.

Abstract

Ultradensification using different types of small cells (SCs) is one of the key enabling solutions to meet the multiple stringent requirements of 5G cellular networks. However, radio resource management (RRM) in ultra-dense heterogeneous networks (HetNets) is not easy due to interferences in multi-tiered architecture and dynamic network conditions. Interferences in 5G HetNets can be efficiently managed only through the techniques which are adaptive and self-organizing to handle dynamic conditions in 5G HetNets. In this article, a machine learning (ML) based self-adaptive resource allocation scheme is proposed based on the combination of independent and cooperative learning and evaluated for ultra-dense 5G HetNets. The proposed scheme aims to improve the QoS of all users associated with different network tiers in ultra-dense HetNets simultaneously. The proposed solution adaptively optimizes the SCs transmit power either through independent learning or cooperative learning based on the varying density of small cells to minimize the interferences and ensure minimum QoS requirements for all users in different network tiers. The proposed scheme not only maintains the minimum required capacities for QoS provision to all users simultaneously but has also shown a significant improvement in the capacities of users in different network tiers in high interference scenarios as compared to the use of a single learning scheme.

Web URL: https://sites2.uol.edu.pk/journals/pakjet/article/view/2393

4. Arshad, R., Farooq-i-Azam, M., Muzzammel, R., Ghani, A., & See, C. H. (2023). Energy efficiency and throughput optimization in 5g heterogeneous networks. Electronics, 12(9), 2031.

Abstract

Device-to-device communication offers a promising technology for the 5G network that aims to enhance the data rate, reduce latency and cost, improve energy efficiency, and provide other desired features. The 5G heterogeneous network (5GHN) with a decoupled association strategy of downlink (DL) and uplink (UL) is a promising solution for the challenges faced in the 4G

heterogeneous network (4GHN). The research presented in this paper evaluates the performance of the 4GHN as well as a DL-and-UL-coupled (DU-CP) access scheme in comparison with the 5GHN with a DL-and-UL-decoupled (DU-DCP) access scheme in terms of the energy efficiency and network throughput in four-tier heterogeneous networks. The energy and throughput are optimized for both scenarios, i.e., DU-CP and DU-DCP, and the results are compared. Detailed performance analyses of the DU-CP and DU-DCP access schemes were conducted with the help of comparisons of the results achieved by implementing a genetic algorithm (GA) and particle swarm optimization (PSO). Both of these algorithms are suited for the non-linear problem under investigation in which the search space is large. The simulation results have shown that the DU-DCP access scheme gives a better performance than the DU-CP scheme in a four-tier heterogeneous network in terms of network throughput and energy efficiency. The PSO achieves an energy efficiency of 12 Mbits/joule for the DU-CP and 42 Mbits/joule for the DU-DCP, whereas the GA yields an energy efficiency of 28 Mbits/joule for the DU-CP and 55 Mbits/joule for the DU-DCP. The performance of the proposed method is compared with those of three other schemes. The results show that the DU-DCP scheme using the GA outperforms the compared methods.

Web URL: https://www.mdpi.com/2079-9292/12/9/2031

5. Iqbal, M. U., Ansari, E. A., Akhtar, S., Farooq-i-Azam, M., Hassan, S. R., & Asif, R. (2023). Optimal learning paradigm and clustering for effective radio resource management in 5G HetNets. IEEE Access.

Abstract

Ultra-dense heterogeneous networks (UDHN) based on small cells are a requisite part of the future cellular networks as they are proposed as one of the enabling technologies to handle coverage and capacity problems. But co-tier and cross-tier interferences in UDHN severely degrade the quality of service due to K-tiered architecture. Machine learning based radio resource management either through independent learning or cooperative learning is a proven efficient scheme for interference mitigation and quality of service provision in UDHN in a both distributive and cooperative manner. However, an optimal learning paradigm selection, i.e., either independent or cooperative learning and optimal cooperative cluster size in cooperative learning for efficient radio resource management in UDHN is still an open research problem. In this article, a Q-learning based radio resource management scheme is proposed and evaluated for both distributive and cooperative schemes using independent and cooperative learning. The proposed Q-learning solution follows the $\epsilon-$greedy policy for optimal convergence. The simulation results for the UDHN in an urban setup show that in comparison to the independent learning paradigm, cooperative learning has no significant impact on macro cell user capacity. However, there is a significant improvement in small cell user capacity and the sum capacity of the cooperating small cells in the cluster. A significant increase of 48.57% and 37.9% is observed in the small cell user capacity, and sum capacity of the cooperating small cells, respectively, using cooperative learning as compared to independent learning which sets cooperative learning as an optimal learning strategy in UDHN. The improvement in small cell user capacity is at cost of increased computational time which is directly proportional to the number of cooperating small cells. To solve the issue of computational time in cooperative

learning, an optimal clustering algorithm is proposed. The proposed optimal clustering reduced the computational time by four times in cooperative Q-learning.

Web URL: https://ieeexplore.ieee.org/abstract/document/10105246

6. Asif, R., Farooq-i-Azam, M., Chaudary, M. H., Husen, A., & Hassan, S. R. (2023). A distance vector hop-based secure and robust localization algorithm for wireless sensor networks. Electronics, 12(10), 2237.

Abstract

Location information of sensor nodes in a wireless sensor network is important. The sensor nodes are usually required to ascertain their positions so that the data collected by these nodes can be labeled with this information. On the other hand, certain attacks on wireless sensor networks lead to the incorrect estimation of sensor node positions. In such situations, when the location information is not correct, the data may be labeled with wrong location information that may subvert the desired operation of the wireless sensor network. In this work, we formulate and propose a distance vector hop-based algorithm to provide secure and robust localization in the presence of malicious sensor nodes that result in incorrect position estimation and jeopardize the wireless sensor network operation. The algorithm uses cryptography to ensure secure and robust operation in the presence of adversaries in the sensor network. As a result of the countermeasures, the attacks are neutralized and the sensor nodes are able to estimate their positions as desired. Our secure localization algorithm provides a defense against various types of security attacks, such as selective forwarding, wormhole, Sybil, tampering, and traffic replay, compared with other algorithms which provide security against only one or two types. Simulation experiments are performed to evaluate the performance of the proposed method, and the results indicate that our secure localization algorithm achieves the design objectives successfully. Performance of the proposed method is also compared with the performance of basic distance vector hop algorithm and two secure algorithms based on distance vector hop localization. The results reveal that our proposed secure localization algorithm outperforms the compared algorithms in the presence of multiple attacks by malicious nodes.

Web URL: https://www.mdpi.com/2079-9292/12/10/2237

7. Farooq-i-Azam, M., Siddiq, A., and M. U. Iqbal, Probability distribution of transient response of an electric circuit.

Abstract

In this work, we explore the transient response of an electric circuit using probabilistic analysis when the precise value of the characteristic parameter of a circuit element is not known and is instead constrained to a range of values. To accomplish this, a combination of probability theory and traditional circuit analysis techniques is employed. In this approach, the circuit element's parameter is treated as a random variable, and probability methods are used to derive the probability distribution of the voltage or current across it. To demonstrate this approach, we apply it to a resistor capacitor (RC) circuit, where the capacitance parameter of the capacitor is regarded as a random variable. We derive probability distributions for the transient voltage

across the capacitor and the voltage at the output terminals to illustrate the method's effectiveness.

Web URL: https://doi.org/10.51846/vol6iss2pp1-8

8. Farooq-i-Azam, M., Khan, Z. H., Ghani, A., & Siddiq, A. (2023). An Investigation of the Transient Response of an RC Circuit with an Unknown Capacitance Value Using Probability Theory. Symmetry, 15(7), 1378.

Abstract

In this research, we investigate a resistor capacitor electric circuit that exhibits an exponentially decaying transient response. Due to uncertainty in the precise capacitance value, we treat the capacitance as a continuous uniformly distributed random variable. Using this approach, we derive the desired transient current response of the circuit as a function of the capacitance. Subsequently, we develop a probability model for the response current, expressed in terms of probability density function and cumulative distribution function. The model's validity and correctness are verified, and it is further utilized for probabilistic analysis of the transient current. We demonstrate the application of the model for determining the probability of the transient current response reaching a specific value. By following the same procedure used to derive the probability model of the transient current, probability distributions for other circuit parameters, such as voltages and currents, can also be obtained. Furthermore, for parameters that are functions of the transient current, the probability model can also be obtained from the already derived probability model. To illustrate this, we derive the probability models of three other parameters in the circuit from the already obtained models. We also present examples to demonstrate the usage of the developed probability models.

Web URL: https://www.mdpi.com/2073-8994/15/7/1378

9. Farooq, M. S., Khalid, H., Arooj, A., Umer, T., Asghar, A. B., Rasheed, J., ... & Yahyaoui, A. (2023). A conceptual multi-layer framework for the detection of nighttime pedestrian in autonomous vehicles using deep reinforcement learning. Entropy, 25(1), 135.

Abstract

The major challenge faced by autonomous vehicles today is driving through busy roads without getting into an accident, especially with a pedestrian. To avoid collision with pedestrians, the vehicle requires the ability to communicate with a pedestrian to understand their actions. The most challenging task in research on computer vision is to detect pedestrian activities, especially at nighttime. The Advanced Driver-Assistance Systems (ADAS) has been developed for driving and parking support for vehicles to visualize sense, send and receive information from the environment but it lacks to detect nighttime pedestrian actions. This article proposes a framework based on Deep Reinforcement Learning (DRL) using Scale Invariant Faster Region-based Convolutional Neural Networks (SIFRCNN) technologies to efficiently detect pedestrian operations through which the vehicle, as agents train themselves from the environment and are forced to maximize the reward. The SIFRCNN has reduced the running time of detecting pedestrian operations from road images by incorporating Region Proposal Network (RPN) computation. Furthermore, we have used Reinforcement Learning (RL) for optimizing the Q-values and training itself to maximize the reward after getting the state from the SIFRCNN. In

addition, the latest incarnation of SIFRCNN achieves near-real-time object detection from road images. The proposed SIFRCNN has been tested on KAIST, City Person, and Caltech datasets. The experimental results show an average improvement of 2.3% miss rate of pedestrian detection at nighttime compared to the other CNN-based pedestrian detectors.

Web URL: https://www.mdpi.com/1099-4300/25/1/135

10. Awan, M. M. A., Asghar, A. B., Javed, M. Y., & Conka, Z. (2023). Ordering Technique for the Maximum Power Point Tracking of an Islanded Solar Photovoltaic System. Sustainability 2023, 15, 3332.

Abstract

The world's attention has turned towards renewable energy due to escalating energy demands, declining fossil fuel reservoirs, greenhouse gas emissions, and the unreliability of conventional energy systems. The sun is the only renewable energy source that is available every day for a specific period of time. Solar photovoltaic (PV) technology is known for its direct conversion of sunlight into electricity using the photoelectric effect. However, due to the non-linear electrical characteristics, the power output of solar PV cells is bound to a lower value and can not produce the power of which it is capable. To extract the maximum possible power, the PV cell needs to be operated at its maximum power point (MPP) uninterruptedly under numerous weather conditions. Therefore, an electronic circuit driven by a set of rules known as an algorithm is utilized. To date, the flower pollination algorithm (FPA) is one of the most renowned maximum power point tracking (MPPT) algorithms due to its effective tracking ability at the local and global positions. After an in-depth analysis of the design, strengths, weaknesses, and opportunities of the FPA algorithm, we have proposed an additional filtration and distribution process named "Random walk" along with the ordering of solutions, to improve its efficiency and tracking time. The proposed structure named "Ordered FPA" has outperformed the renowned FPA algorithm under various weather conditions at all the standard benchmarks. Simulations are performed in MATLAB/Simulink.

Web URL: https://www.mdpi.com/2071-1050/15/4/3332

DEPARTMENT OF ENERGY RESEARCH CNETER

1. Azeem, F., Memon, Z. A., Baig, S., Manzoor, T., Abbas, F., & Shah, M. A. (2023). A novel automated demand response control using fuzzy logic for islanded battery-operated rural microgrids. IET Renewable Power Generation, 17(7), 1797-1811.

ABSTRACT:
Islanded rural microgrid require continuous resource monitoring. Demand response schemes have been phenomenal in managing loads. However, urban demand response schemes are well equipped with market prices and peak time penalties to control deferrable loads. In rural microrids, regular loads such as fans, lights and water pumps are normally used that do not fall under category of deferrable loads. In addition, full liberty of utilizing regular load at any time, lack of awareness and no information of storage reserves make task of load management more complex. In this research fully automated two layered demand response scheme is designed for regular operating loads. The first layer control is load mode control. The mode of operation is decided on the state of charge (SoC) of battery. In second layer, fuzzy controller is designed on the consumer's routines, SoC and ambient temperature as membership function. Results are assessed in terms of consumers comfort and availablity of SoC. The load operation in automated demand response remained indentical to actual rutine operation as per consumer's desire with 5 to 7% deviation. In all modes of operation SoC levels remained 15% higher and heavy load operated 13.5% more compare to relevant study.

Web URL: https://ietresearch.onlinelibrary.wiley.com/doi/full/10.1049/rpg2.12713

2. Azeem, F., Memon, Z. A., Baig, S., & Awan, A. B. (2023). A two-way pre-installation assessment framework for microgrids under power systems expansion planning. Sustainable Energy Technologies and Assessments, 55, 102920.

ABSTRACT:
Many remote areas remain off the grid and are disconnected from the mainstream power network due to congestion in the existing power networks and expensive expansion plans. In recent studies, microgrid installations appeared as one of the most feasible solutions for power system expansion. This research study develops a two-way (M to G), where the existing microgrid is integrated into the distribution network, and (G to M) where distribution system expansion recommends the installation of a microgrid. The proposed framework is based on three steps. The initial assessment is based on a fuzzy assessment tool utilizing social factors,

geographic location, and accessibility followed by economic feasibility analyses. These analyses are based on HOMER software and a power flow study of the microgrid to assess the system's reliability. The proposed framework is implemented on an islanded microgrid in a village in Pakistan. The acquired results have shown that the proposed framework recommends the existing microgrid expansion in M to G mode. The Net Present Cost (NPC) of the grid-connected system is reduced from $11 million to $0.7 million. The cost of energy is also reduced to $4.42 compared to the $65 of the islanded systems, while the payback period is only 1.2 years compared to that of the islanded microgrid which is 8.6 years.

Web URL: https://www.sciencedirect.com/science/article/pii/S2213138822009687

3. Moreira, T. F., Camponogara, Â., Baig, S., & Ribeiro, M. V. (2023). Performance analysis of orthogonal multiplexing techniques for PLC systems with low cyclic prefix length and symbol timing offset. Sensors, 23(9), 4363.

ABSTRACT:
This paper investigates the degradation caused by interference resulting from cyclic prefix violation and symbol timing offset in narrowband power line communication systems. In this sense, it presents a unified formulation from which Hermitian symmetric orthogonal frequency division multiplexing (HS-OFDM), orthogonal chirp division multiplexing (OCDM), single-carrier cyclic prefix (SCCP), and orthogonal time–frequency division multiplexing (OTFDM) can be easily derived. The paper then provides closed-form expressions for quantifying the aforementioned interference in the presence of a frequency domain equalizer. The numerical analyses exhibit the performances of these schemes under various data communication conditions, such as the availability of channel state information, the presence or absence of interference, modeling of additive noise as a white or colored Gaussian random process, frequency domain equalizer type, and the use of bit and power allocation techniques. The closed-form expressions and performance analyses regarding achievable data rate and bit error probability provide guidance for dealing with distinct constraints in narrowband power line communication (PLC) systems using the HS-OFDM, OCDM, SCCP, or OTFDM scheme. Lastly, the unified formulation and results obtained motivate the design of multi-scheme transceivers.

Web URL: https://www.mdpi.com/1424-8220/23/9/4363

4. Farooq, S., Manzoor, T., Siddiqui, A. A., & Arslan, M. (2023). Numerical Analysis of Hartmann Number Influence on Nonlinear Horizontal Stretched Sheet. Southern Journal of Engineering & Technology, 1(01), 10-20.

ABSTRACT:
This study examines numerically the problem of Hartmann number influence on two medium conduction-convection (conjugate) flow of nanofluids on a nonlinear horizontal stretched sheet. This model nonlinear partial differential equation solved by using Keller box method for nanofluid integrates the influence take on the buoyancy parameter, solute buoyancy, Brownian

motion, thermophoresis parameter, Prandtl number and Lewis number found to have a strong effect on the system. The numerical result showed the velocity profile decreases during Prandtl number increases and temperature of Nano fluid increases under the influence of Hartmann number. The reduced Nusselt number when Prandtl number rises and reduced Sherwood number for large values of Lewis number. The Hartmann number influence and different parameters are presented through table and graph.

Web URL: https://sjet.isp.edu.pk/index.php/sjet/article/view/6

5. Manzoor, T., Gohar, G. A., Asghar, A., & Manzoor, S. (2023). Analysis of vertical axis wind turbine blade for off-shore applications. Wind Engineering, 47(3), 499-514.

ABSTRACT:

In this work, static and dynamic analyses are carried out on VAWT blade using analytical and numerical methods to figure out reasons behind the failure in the blade for off-shore applications arising due to turbulence of wind. The design flaws and different operating conditions play major role in failure of blades. Fatigue life cycles, natural frequencies of blade in different modes and turbine harmonic frequency have been calculated analytically using Goodman's and vibration analysis theories respectively. In analysis, life cycles, natural frequencies and mode shapes for VAWT blade are studied. Analytical and numerical results have been compared, life cycles and frequencies are determined. The numerical results showed good agreement with theoretical concepts.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/0309524X221131999

6. Sipra, A. T., Azeem, F., Memon, Z. A., Baig, S., & Jaffery, M. H. (2024). Design and assessment of energy management strategy on rail coaches using solar PV and battery storage to reduce diesel fuel consumption. ***Energy*****,** ***288*****, 129718**.

ABSTRACT:

This study is focused to develop energy management strategy using battery backup source for electrical load of the rail coaches. To assess the effectiveness of battery storage inclusion, the higher and lower battery state of charge cases were simulated using parametric approach where solar Photovoltaic (PV) power, battery state of charge (SoC) and load consumption parameters were used develop the controller. Fuzzy logic and Adaptive neuro-fuzzy interference system (ANFIS) approaches were used for the controller design. It was found that the Solar PV-battery hybrid system helps in a significant reduction in diesel consumption i.e., about 10 % in diesel savings with higher SoC values and 7 % of diesel savings during worst cases. Annually, while comparing two controllers, it was found that the annual diesel savings increase from PKR 604.17 million to PKR 684.00 million, while the amount of CO_2 emissions reduction increase from 6932.70 to 7848.75 tons, while using ANFIS control.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360544223031122

7. Hassan, B., Baig, S., & Aslam, S. (2023). On Scalability of FDD-Based Cell-Free Massive MIMO Framework. *Sensors*, *23*(15), 6991.

ABSTRACT:

Cell-free massive multiple-input multiple-output (MIMO) systems have the potential of providing joint services, including joint initial access, efficient clustering of access points (APs), and pilot allocation to user equipment (UEs) over large coverage areas with reduced interference. In cell-free massive MIMO, a large coverage area corresponds to the provision and maintenance of the scalable quality of service requirements for an infinitely large number of UEs. The research in cell-free massive MIMO is mostly focused on time division duplex mode due to the availability of channel reciprocity which aids in avoiding feedback overhead. However, the frequency division duplex (FDD) protocol still dominates the current wireless standards, and the provision of angle reciprocity aids in reducing this overhead. The challenge of providing a scalable cell-free massive MIMO system in an FDD setting is also prevalent, since computational complexity regarding signal processing tasks, such as channel estimation, precoding/combining, and power allocation, becomes prohibitively high with an increase in the number of UEs. In this work, we consider an FDD-based scalable cell-free network with angular reciprocity and a dynamic cooperation clustering approach. We have proposed scalability for our FDD cell-free and performed a comparative analysis with reference to channel estimation, power allocation, and precoding/combining techniques. We present expressions for scalable spectral efficiency, angle-based precoding/combining schemes and provide a comparison of overhead between conventional and scalable angle-based estimation as well as combining schemes. Simulations confirm that the proposed scalable cell-free network based on an FDD scheme outperforms the conventional matched filtering scheme based on scalable precoding/combining schemes. The angle-based LP-MMSE in the FDD cell-free network provides 14.3%14.3% improvement in spectral efficiency and 11.11%11.11% improvement in energy efficiency compared to the scalable MF scheme.

Web URL: https://www.mdpi.com/1424-8220/23/15/6991

8. Azeem, F., Irshad, B., Zidan, H. A., Narejo, G. B., Hussain, M. I., & Manzoor, T. (2023). Design and Analysis of a Peak Time Estimation Framework for Vehicle Occurrences at Solar Photovoltaic and Grid-Based Battery-Swappable Charging Stations. *Sustainability*, *15*(23), 16153.

ABSTRACT:

Due to global environmental impacts, the electric vehicle (EV) adoption rate is increasing. However, unlike conventional petrol vehicles, EVs take a considerable time to charge. EVs on the road with different battery charging statuses and driving demographics may cause uncertain peak time arrivals at charging stations. Battery-swappable charging stations are a quick and easier way to replace uncharged batteries with charged ones. However, charging due to uncertain EV arrival causes higher charging profiles posing load to the grid, management of charged and discharged batteries, and peak time charging tariffs. These challenges hinder the wide operation of battery-swappable charging stations. Nevertheless, a pre-assessment of peak hours using EV demographics can reduce congestion. In recent literature surveys for battery-swappable charging stations, spot congestion has not been given much attention, which has a direct influence on the

sizing and operation of battery-swappable charging stations. This research study is focused on estimating peak time events using a novel integrated techno-economic assessment framework. A fuzzy-based parametric assessment tool is developed that identifies the factors that influence higher congestion events. Based on the peak event assessment, grid, and solar PV-based generation is optimized using mixed integer linear programming. In the final step, an environment analysis of a swappable charging station is performed. Furthermore, the results achieved using the proposed framework for battery-swappable charging stations (BSCSs) were compared with fast-charging (FC) stations. FC can economically perform well if integrated with solar PV systems; however, the capital cost is 80% greater than the BSCSs designed under the proposed framework. The operational cost of BSCSs is 39% higher than FC stations as they use 29% higher grid units than FC stations due to night operations under congestion

Web URL: https://www.mdpi.com/2071-1050/15/23/16153

9. Al-Atawi, A. A., Alyahyan, S., Alatawi, M. N., Sadad, T., Manzoor, T., Farooq-i-Azam, M., & Khan, Z. H. (2023). Stress Monitoring Using Machine Learning, IoT and Wearable Sensors. *Sensors*, *23*(21), 8875.

ABSTRACT:

The Internet of Things (IoT) has emerged as a fundamental framework for interconnected device communication, representing a relatively new paradigm and the evolution of the Internet into its next phase. Its significance is pronounced in diverse fields, especially healthcare, where it finds applications in scenarios such as medical service tracking. By analyzing patterns in observed parameters, the anticipation of disease types becomes feasible. Stress monitoring with wearable sensors and the Internet of Things (IoT) is a potential application that can enhance wellness and preventative health management. Healthcare professionals have harnessed robust systems incorporating battery-based wearable technology and wireless communication channels to enable cost-effective healthcare monitoring for various medical conditions. Network-connected sensors, whether within living spaces or worn on the body, accumulate data crucial for evaluating patients' health. The integration of machine learning and cutting-edge technology has sparked research interest in addressing stress levels. Psychological stress significantly impacts a person's physiological parameters. Stress can have negative impacts over time, prompting sometimes costly therapies. Acute stress levels can even constitute a life-threatening risk, especially in people who have previously been diagnosed with borderline personality disorder or schizophrenia. To offer a proactive solution within the realm of smart healthcare, this article introduces a novel machine learning-based system termed "Stress-Track". The device is intended to track a person's stress levels by examining their body temperature, sweat, and motion rate during physical activity. The proposed model achieves an impressive accuracy rate of 99.5%, showcasing its potential impact on stress management and healthcare enhancement

Web URL: https://www.mdpi.com/1424-8220/23/21/8875

10. Hassan, B., Baig, S., Aslam, S., Asif, H. M., & Mumtaz, S. (2024). Adaptive refined random orthogonal matching pursuit algorithm for FBMC/OQAM MIMO framework. *Alexandria Engineering Journal*, *87*, 319-328.

ABSTRACT:

The fifth generation of wireless communication is anticipated to provide improved quality of service and enhanced data rates to the end users. One such technology that stands out as a potential transmission scheme for 5G systems is Filter Bank Multicarrier using Offset Quadrature Amplitude Modulation (FBMC/OQAM) with an effective channel estimation technique for improved performance. However, due to the inherent imaginary interference, channel estimation methods relying on preamble structures in FBMC/OQAM systems exhibit sub-optimal performance, particularly within Multiple-Input Multiple-Output (MIMO) setups. For channel estimation schemes based on compressed sensing, the inherent sparsity of wireless channels can be exploited for accurate channel reconstruction and overall performance improvement.
We propose a novel compressed sensing based algorithm namely, Adaptive Refined Random Orthogonal Matching Pursuit (ARROMP), for MIMO-FBMC system with Coordinated MultiPoint (CoMP) scheduling. This algorithm adaptively selects a support set by utilizing a double threshold for the minimization of mean squared error and for accurate channel reconstruction. The proposed algorithm's performance is compared with existing Orthogonal Matching Pursuit (OMP) schemes such as random OMP, refined random OMP, and least square-based estimation. The numerical simulations suggest that the proposed adaptive algorithm provides performance improvement in terms of reduced Mean Squared Error (MSE) of channel reconstruction and Bit Error Rate (BER). Moreover, the proposed ARROMP algorithm for MIMO-FBMC is rigorously tested with CoMP scheduling for a cellular network using frequency division duplex mode. The proposed system presents significant improvements in throughput and spectral efficiency for all types of cell users, including cell-edge users. The simulation results validate the improved performance of the proposed algorithm with CoMP scheduling over the existing single-cell system with no coordination.

Web URL: https://www.sciencedirect.com/science/article/pii/S1110016823011183

11. Mouhy-Ud-Din, M. A., Azeem, F., Memon, Z., & Arshad, J. (2024). Comparative techno-economic assessment of electric vehicle charging preferences: A quantitative study for sustainable EV policy in Pakistan. *Energy for Sustainable Development*, *78*, 101355.

ABSTRACT:

Sustainable induction of Electric vehicles (EV) adoption in developing countries requires a comprehensive policy and planning. Among several challenges, one of the biggest challenges is a sustainable charging station infrastructure integration to the existing weak distribution power network. Based on technological advancements, EV owners enjoy better milage in one charge. This has given a liberty to charge EVs as per the desire of user. There are two kinds of charging preferences, one is home charging and the other is fast charging. Both charging choices have distinct economic and technical aspects that need to be quantified in line with the available power infrastructure so as to develop a policy regulation. This study aims to quantitatively assess home charging, level 3 fast charging and their techno-economic aspects using social demographics of car owners. To analyze the demographics of local vehicle mobility practices in Pakistan, a comprehensive survey comprising online questionnaire was conducted. >100 car owners were surveyed about their daily driving practices to understand the driving distances and their preference of charging vehicles. The driving owners from distinct occupations ranging from cab drivers, job holders and businessmen participated in the survey. The survey facilitated to

identify the demographics of the car owners which helped in conducting simulations and quantification analysis. Monte Carlo simulation was used for 1000 cars samples to estimate the level 1 and level 3 charging profiles in Python. In second step, HOMER Grid software was used to economically assess the impact of home charging and fast charging. It was revealed that charging choices have significant impact on the daily load profile of EVs. While having home charging, 59.9 % higher units are purchased from the grid. Whereas 65.5 NPC is increased for the project. On the other hand, the daily profile of preferred home charging is 61.4 % higher compared to the fast charging due to much concentrated charging impact during the limited time of the day. Results highlighted that Solar PV plays an important role for fast and home charging. Without solar PV charging stations will consume 60 % more grid units and 58 % higher Net present cost. The study concludes with a set of policy recommendations that must be taken into account to support the weak grid and lessen the EV charging impact on main utility.

Web URL: https://www.sciencedirect.com/science/article/pii/S0973082623002120

12. Arshad, R., Baig, S., & Aslam, S. (2024). User clustering in cell-free massive MIMO NOMA system: A learning based and user centric approach. Alexandria Engineering Journal, 90, 183-196.

ABSTRACT:

For future wireless communications, Cell-free Massive Multiple-Input Multiple-Output (CF-mMIMO) systems and Non-orthogonal Multiple Access (NOMA) schemes are considered potential candidates to meet the greater coverage and capacity demands. Nevertheless, a traditional CF-mMIMO system faces scalability issues and poses numerous challenges in handling the expanding number of user equipment and ensuring their dependable connectivity, particularly in larger geographical areas. To address this challenge, a user-centric (UC) approach is implemented in a CF-mMIMO system, wherein a designated subset of access points (APs) serves a specific number of users from the entire pool of available APs. To implement a NOMA aided CF-mMIMO system, users must be grouped using a suitable clustering scheme to achieve greater spectral efficiency (SE), sum-rate, and reduced bit error rate (BER). For efficient user clustering, unsupervised machine learning (ML) algorithms, such as k-means, k-means++, and improved k-means++ are employed. In this paper, a multiuser NOMA aided CF-mMIMO system with a UC approach is investigated and closed-form expressions for intra-cluster interference and SINR are derived and the performance of the proposed system is analyzed in terms of achievable sum-rate and BER. The proposed system with the UC approach and three ML algorithms namely k-means, k-means++, and improved k-means++ demonstrate 12%, 10%, and 17% higher achievable sum-rate as compared to the NUC approach with same ML algorithms respectively. Similarly, the proposed system with UC and ML approaches exhibits 52%, 55% and 61% improved achievable sum-rate respectively, as compared to far pairing, random pairing, and close pairing schemes. Moreover, the system model is validated through the conformity of the theoretically derived bit error rate with the simulation results for a three-user scenario

Web URL: https://www.sciencedirect.com/science/article/pii/S1110016824000863

13. Anwar, T., Manzoor, T., Hussain, N., Shah, S. N., Perveen, S., Asif, S. U., ... & Manzoor, H. U. (2024). Antimony Trisulfide with Graphene Oxide Coated Titania

Nanotube Arrays as Anode Material for Lithium-ion Batteries. Journal of Inorganic and Organometallic Polymers and Materials, 1-8.

ABSTRACT:

The performance of the Lithium Ion Batteries (LiBs) is significantly influenced with the synergetic chemical properties of two different materials in a composite form. The specific capacity of both titanium dioxide arrays (TNAs) and Antimony trisulfide (Sb_2S_3) bottleneck the performance of LiB due to the low conductivity after the implantation as anode material. Herein, a novel multifunctional composite composed of highly dispersed Sb_2S_3 on freestanding tubular TNAs host via chemical bath deposition method (CBD) for use as anode material in lithium-ion batteries (LIBs). The loading quantity of Sb_2S_3 with reduced graphene oxide (rGO) was regulated to achieve adjustable outcomes. The composite anode consisting of TNAs/ Sb_2S_3/G in lithium-ion batteries (LIBs) has a specific capacity that is three times greater than conventional anodes. Furthermore, this composite anode maintains stable cyclic performance even after undergoing 300 cycles. The initial coulombic efficiency of the composite electrode is 100%, whereas the bare TNAs had a coulombic efficiency of 45%. The cycle performance analysis demonstrated that the TNAs/ Sb_2S_3/G composite has superior specific capacity and efficiency, evenunder high current density conditions of 500 $\mu A/cm^2$. The rate performance is greatly improved, indicating the efficacy of this innovative composite anode material for high-performance LIBs.

Web URL: https://link.springer.com/article/10.1007/s10904-024-03135-y

14. Manzoor, H. U., Manzoor, S., Jamshed, M. A., & Manzoor, T. (2024). Leveraging InGaN solar cells for visible light communication reception. *IET Networks*.

ABSTRACT:

Solar cells are increasingly being utilised for both energy harvesting and reception in free-space optical (FSO) communication networks. The authors focus on the implementation of a mid-band p-$In_{0.01}Ga_{0.99}$ N/p-$In_{0.5}Ga_{0.5}$ N/n-$In_{0.5}Ga_{0.5}$ N (PPN) solar cell, boasting an impressive 26.36% conversion efficiency (under 1.5AM conditions) as a receiver within an indoor FSO communication network. Employing a solar cell with dimensions of 1 mm in length and width, the FSO system underwent simulation using Optisystm software, while the solar cell's behaviour was simulated using SCAPS-1D. The received power from the solar cell was then compared to that of four commercially available avalanche photodiode (APD) receivers. Exploring incident wavelengths spanning 400–700 nm within the visible spectrum, across transmission distances of 5, 10, 15, and 20 m, the study presented current-voltage (IV) and power-voltage curves. Notably, the InGaN solar cell exhibited superior electrical power output compared to all commercial APDs. In conclusion, the findings underscore that augmenting received power has the potential to enhance FSO network quality and support extended transmission distances.

Web URL: https://ietresearch.onlinelibrary.wiley.com/doi/full/10.1049/ntw2.12115

15. Manzoor, T., Zahid, M. A., Manzoor, S., Hussaian, M., Azeem, F., Ahmed, U., & Manzoor, H. U. (2024). Analysis of shape memory alloys' strain energy absorption dampers: RTDM approach. Crystals.

ABSTRACT:

Enlighten (hereafter referred to as 'website') is run by the University of Glasgow.

We want as many people as possible to be able to use this website. For example, that means you should be able to:

- change colours, contrast levels and fonts
- zoom in up to 300% without the text spilling off the screen
- navigate most of the website using just a keyboard
- navigate most of the website using speech recognition software
- listen to most of the website using a screen reader (including the most recent versions of JAWS, NVDA and VoiceOver)

We have also made the text in the website as simple as possible to understand and have implemented additional accessibility features where possible.

Web URL: https://www.gla.ac.uk/legal/accessibility/statements/enlighten/

16. Sipra, A. T., Azeem, F., Memon, Z. A., Baig, S., & Jaffery, M. H. (2024). Design and assessment of energy management strategy on rail coaches using solar PV and battery storage to reduce diesel fuel consumption. *Energy*, *288*, 129718.

ABSTRACT:

This study is focused to develop energy management strategy using battery backup source for electrical load of the rail coaches. To assess the effectiveness of battery storage inclusion, the higher and lower battery state of charge cases were simulated using parametric approach where solar Photovoltaic (PV) power, battery state of charge (SoC) and load consumption parameters were used develop the controller. Fuzzy logic and Adaptive neuro-fuzzy interference system (ANFIS) approaches were used for the controller design. It was found that the Solar PV-battery hybrid system helps in a significant reduction in diesel consumption i.e., about 10 % in diesel savings with higher SoC values and 7 % of diesel savings during worst cases. Annually, while comparing two controllers, it was found that the annual diesel savings increase from PKR 604.17 million to PKR 684.00 million, while the amount of CO_2 emissions reduction increase from 6932.70 to 7848.75 tons, while using ANFIS control.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360544223031122

17 Sarfraz, A., Usman, M., Hussain, N., Shafaat, S., Khan, A. M., Hussain, Z., ... & Shaikh, A. J. (2024). A Pathway to Optimal Multivariate Synthesis of Fe2O3-CuO Bimetal Oxide Hybrid Nanoparticles: Transformation Through Mathematical Modelling. *JOM*, 1-20.

ABSTRACT:

Controlled and multivariate synthesis of Fe_2O_3-CuO bimetallic oxide nanoparticles is achieved by coprecipitation method with different concentrations of iron and copper oxide, followed by their optimization at specific pH, temperature, and time of addition of reagent. Concentration

studies revealed changes in spectral band position to a hyperchromic shift with relevant increase in the concentration of CuO (100%). Hybrids with higher CuO concentration lead to hybrids with smaller size and higher stability. Temperature-dependent synthesis of bimetallic hybrid oxide nanoparticles showed an increase in size at higher temperatures, while at lower temperatures, stable oxide particles are observed. For pH-dependent synthesis, controlled size is observed at higher pH. Increasing the time of addition of reactant for optimized synthesis of bimetallic oxide nanoparticles showed a gradual decrease in size, hence better control. The results of size and zeta potential are transformed by the application of probability distribution function and grow-decay model.

Web URL: https://link.springer.com/article/10.1007/s11837-024-06423-7

18. Usman, M., Sarfraz, A., Shafaat, S., Hussain, N., Khan, A. M., Hussain, Z., ... & Shaikh, A. J. (2024). A multiparametric study for size and stability of hybrid Fe2O3-NiO nanoparticles and their statistical transformation. *Particulate Science and Technology*, 1-20.

ABSTRACT:

Bimetallic mixed metal oxide hybrid nanoparticles of iron and nickel are prepared via the co-precipitation method and are characterized by various techniques. Optimization of these nanoparticles involves finding the optimal synthetic conditions and parameters to achieve the hybrid material's desired size, stability, and composition. The effects of the ratio of precursor salts, time of addition of reactant, pH, and the temperature for the synthesis of these mixed oxide nanoparticles are investigated. Concentration studies revealed successful synthesis of the hybrids with the controlled smallest size, at equal concentrations of precursor salts. pH and time of addition of reactant studies revealed the synthesis of least-sized hybrids at pH 13 and at a slow mode of addition of reactant. The optimal temperature at which hybrid nanoparticles are found at the smallest controlled size is 40 °C, whereas increasing temperature causes an increase in the size of nanoparticles. The hydrodynamic size and zeta potential studies are also evaluated through statistical models including probability distribution function and grow-decay model, revealing optimized points in terms of probability and the growth or decay of slopes. These studies can potentially demonstrate the optimized potential of these nanoparticles for a variety of applications including energy storage, catalysis, sensing, etc.

Web URL: https://www.tandfonline.com/doi/full/10.1080/02726351.2024.2347835#abstract

DEPARTMENT OF HUMANITIES

1. Muazzam, A., Naseem, F., Shakil, M., Visvizi, A., & Klemens, J. (2023). Surviving COVID-19: Biopsychosocial Impacts, Death Anxiety, and Coping Strategies. Vaccines 2023, 11, 705.

ABSTRACT:
As the COVID-19 pandemic erupted, attempts to contain the spread of the virus took two concurrent forms, including mobility restrictions (aka lockdowns) and the race to produce a vaccine. However, it is quite striking that, amidst both the lockdown and the race to produce a vaccine, the question of how COVID-19 survivors/patients coped with the disease has not received the degree of attention it deserved. To navigate this issue, we employed a sample consisting of 100 COVID-19 survivors; this paper explores the relationship between the biopsychosocial (BPS) impacts of COVID-19, death anxiety, and coping strategies. In this context, the mediating role of death anxiety is placed in the spotlight. The analysis reveals a significant positive association between the BPS impact of COVID-19 and death anxiety and a significant negative association between death anxiety and coping strategies among COVID-19 survivors. Thus, death anxiety mediates the relationship between the BPS impact and the coping strategies that COVID-19 survivors adopt. Given the general recognition of the validity of the BPS model in contemporary medical science and practice, a thorough examination of COVID-19 survivors and their experiences related to surviving is necessary to match the challenges of today, including the increased probability of pandemics.

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2. Khan, S., & Anjum, M. A. I. (2023). Words in Mental Lexicon: A Comparative Analysis of Word Association (WA) Responses of Pakistani L1 and Afghan L2 Speakers of Urdu. Journal of Communication and Cultural Trends, 5(1), 86-105.

ABSTRACT:
Vocabulary acquisition in both L1 and L2 has depended on the opinion of associative language learning to help recognize and elucidate the procedures of lexical acquisition and development in the mind of language learners. To date, L2 studies in this area have delivered relatively controversial findings. The current study revisited certain corresponding issues in order to gain insight into the restoration of words in the mental lexicon. Moreover, it also strived to understand the relationship between lexical development and the process of word association (WA). To better understand the relationship between lexical meaning and mental lexicon, this study explored and compared the word associations of a group of Afghan Urdu speakers and a group of Urdu native speakers. It aimed to understand how mental links are developed between lexical items in the mental lexicon, a process commonly believed to partially support vocabulary acquisition. The findings revealed that paradigmatic relations created by L2 learners are dominant in their data sets, while syntagmatic relations are leading in L1 data sets. The findings support general trends in this area of research, that is, learning of Urdu language in Pakistan by foreigners. Moreover, the findings further highlight the importance of lexical associative processes employed in second language acquisition. To conclude, the study contributes to WA research, the description of mental lexicon, and L2 language learning and teaching

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3. Ahmad, T., & Ullah, S. (2023). Development Under Belt and Road Initiative: Gains for Tourism Industry in Participant Countries. Journal of China Tourism Research, 19(4), 950-972.

ABSTRACT:
BRI is a mega-development project covering 140 countries in three continents; Asia, Africa, and Europe. The political and economic dimensions of BRI have been studied in several studies in the literature, but the effect on tourism has been less explored. Tourism development has been

linked with sustainable development goals due to its substantial economic potential. A panel dataset of 151 countries from 2000–2019 is used to analyze the effect of participation in BRI on the tourism industry. The PSM-DID model is used after testing the validity through the event-study approach. The robustness of the estimates was tested through counterfactual evidence and a placebo test. The findings show that participation in BRI has increased the number of inbound tourists by 18.4% and tourism revenues by 7%. BRI proved relatively more beneficial for the tourism industry of South Asian, Western Asian, and Middle Eastern countries. The regional difference can be attributed to tourist attraction spots, entry regulations for foreigners, the service quality of the tourism industry, and support facilities offered to tourists. The cooperation among the countries should be increased to facilitate tourists. Tourism companies can use these findings to improve their selection of target markets and future development plans.

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DEPARTMENT OF IRCBM

1. Suhail, F., Batool, M., Anjum, T., Shah, A. T., Tabassum, S., Khan, A. L., ... & Gilani, M. A. (2023). Enhanced CO2 separation performance of polysulfone membranes via incorporation of pyrazole modified MCM-41 mesoporous silica as a nano-filler. Fuel, 350, 128840.

ABSTRACT:
Polymeric membranes are one of the widely used materials of choice for CO_2 capture from major industrial sources. However, the current generation of polymeric materials are unable to keep up with the increasing separation needs of CO_2 from the air (CO_2/N_2) or natural gas (CO_2/CH_4) on an industrial scale due to their so-called permeability-selectivity tradeoff. In an effort to improve the overall gas separation performance of polymeric membranes, mixed matrix membranes (MMMs) have been suggested as a substitute strategy. In this study, Polysulfone (PSf) based MMMs were prepared by incorporating pyrazole modified MCM-41 mesoporous silica (MP) as a nano-filler in the polymer matrix to enhance the gas separation properties of membranes. MCM-41 nano-filler was synthesized and functionalized by post-grafting technique to prepare the MMMs of three different loadings (10, 20, and 30 wt%). All the membranes were characterized for physical, chemical, and thermal analysis. The CO_2 gas separation performance of membranes was assessed, and the results concluded that the MCM-41-based MMMs showed the tradeoff between permeability and selectivity in the case of ideal and mixed gases. This permeability-selectivity trade-off is solved by the MP-based MMMs due to the presence of CO_2-philic functional groups present on the surface of membranes. The PSf-MP membrane with the highest nanofiller loading (30 wt%) showed 79% more permeability than the pure PSf membrane. Additionally, it showed a significant enhancement of 33% and 51% in ideal selectivity for CO_2/CH_4 and CO_2/N_2, respectively, compared to pure PSf membrane. These findings support the lack of membrane faults, the enhanced filler/polymer interface, and the remarkable nano-filler dispersion in the polymer matrix. The excellent outcomes demonstrated the potential of these membranes for more industrial gas separation applications.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0016236123014539**

2. Khan, A. S., AlDahlan, B. G., Maghrabi, N. H., Albilali, H. W., Ahmed, S. Z., Shah, A. T., ... & Talal, A. (2023). Application of laser on enamel surface with three types of bioactive glasses-based resin infiltrants: an in vitro study. Journal of the Mechanical Behavior of Biomedical Materials, 141, 105792.

ABSTRACT:
Objective

The study aimed to evaluate and compare the surface micro-hardness, roughness, color, and morphology of enamel after Er,Cr:YSGG laser irradiation, followed by application of three types of bioactive glasses-based resin infiltrants, and the samples groups were challenged with the pH cycle.

Methodology

Experimental photoactivated resin infiltrants were synthesized using dimethacrylate resins, whereby three different types of bioactive glasses (BGs), i.e., 45S5, fluoridated-BG (F-BG), and borosilicate-BG (B-BG), were incorporated into the resin system. Initially, white spot lesions were created artificially on the toosth enamel surface, then irradiated with Er,Cr:YSGG laser. Then, the resin-only and BG-based resins were infiltrated on the enamel surface. All samples were pH challenged for 14 days, and the micro-hardness, surface roughness, surface morphology, and color stability (ΔE) analyses were conducted before and after the 14 days pH challenge.

Results

After laser irradiation, the micro-hardness was significantly high with 45S5 group compared to resin-only ($p = 0.021$), F-BG ($p = 0.042$), and B-BG ($p = 0.001$) groups. After the pH challenge, the micro-hardness values for all groups were reduced significantly ($p \leq 0.05$). The surface roughness was least with the resin-only group and showed a non-significant difference with F-BG ($p = 0.34$) and significant differences with both B-BG ($p = 0.005$), and 45S5 ($p = 0.010$) groups. After the pH cycle, the roughness of all groups was increased significantly ($p \leq 0.05$), except B-BG group showed a non-significant difference ($p = 0.528$). The B-BG group showed significantly high ΔE between day 0 and baseline compared to resin-only ($p = 0.0008$), F-BG ($p = 0.017$), and 45S5 ($p = 0.029$), whereas between day 14 and baseline, the lowest ΔE value was observed for B-BG (14.2 ± 2.10) and maximum for the resin-only (20.57 ± 2.47) group. The SEM images showed pitting on the surface of all resin infiltrant groups after 14 days of pH challenge.

Conclusion

The morphological difference was observed after the laser irradiation on the enamel surface. The differences in micro-hardness, surface roughness, and color were observed after the application of experimental resin infiltrants and significant differences were observed after the pH challenge.

Web URL: https://www.sciencedirect.com/science/article/pii/S1751616123001455

3. Hassan, A., Mattioli, I. A., Colombo, R. N., & Crespilho, F. N. (2023). Tuning quantum capacitance in 2D graphene electrodes: the role of defects and charge carrier concentration. Journal of Materials Chemistry C, 11(19), 6301-6305.

ABSTRACT:

Even though graphene has been intensively applied in electrochemical devices, the effects of oxidation and how the presence of graphene structural defects interferes with the monolayer graphene electrode–aqueous electrolyte interface remains unclear. Here, we investigate the role of structural defects in the quantum capacitance at the interface between a graphene monolayer and the aqueous electrolyte solution, where the graphene was gradually oxidized by a temporal-controlled electrochemical procedure. We show that the quantum capacitance of graphene can be modulated by tuning the electronic properties, which resulted in a three-fold increase from a

value of 3.83 μF cm^{-2} for the pristine graphene up to 11.11 μF cm^{-2} for the structurally modified monolayers. A strong correlation is observed between the carrier concentration, density of defects, and quantum capacitance. We suggest that the control of such properties can modulate the performance of graphene-based electrochemical devices according to application.

Web URL: **https://pubs.rsc.org/en/content/articlelanding/2023/tc/d2tc04037a/unauth**

4. Akram, M., Shi, J., Khalid, H., Zeng, F., & Tian, Y. (2023). Morphological effect of fabricated surfaces obtained from fluorinated porphyrin based copolymer for oxygen and pressure sensing applications. European Polymer Journal, 192, 112081.

ABSTRACT:
Good oxygen sensitivity and fast response of oxygen probe is primary requirement for pressure sensing applications. Therefore in this study, porphyrin based new fluorinated oxygen probe (OP) monomer was synthesized and copolymerized with 2-(3-(6-methyl-4-oxo-1,4-dihydropyrimidin-2-yl)ureido)ethyl methacrylate (SCMHBMA), octafluoropentyl methacrylate (OCFPM) and butyl acrylate (BA). SCMHBMA may play important biological role in cell adhesion. OCFPM and BA were used as fluorinated and non-fluorinated monomers, respectively. The synthesized oxygen sensitive copolymer (OSC) was used to fabricate spin coated film and membranes of electrospun beaded nanofibers and only nanofibers. Morphological effect of fabricated surfaces was evaluated in terms of oxygen sensitivity, response time and pressure sensitivity. The surface of beaded nanofibers was considered transition state between plain spin coated films surface and fibrous membrane. Nanofibers membrane showed highest oxygen sensitivity (I_0/I 36.7) and pressure sensitivity (0.92 %) among all the surfaces. Moreover, nanofibers membrane exhibited fast response to oxygen ($t_{95\%}$ 0.6 s). Moreover, the electrospun nanofiber membrane was found biocompatible by inherent culture of HeLa cells. Hence, the fabricated membranes may find applications in pressure mapping of biological systems and unsteady surfaces.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0014305723002641**

5. Abid, S., Zulfiqar, S., Anjum, M. A., Bullock, A. J., MacNeil, S., & Yar, M. (2023). An alginate-Based tube gel delivering 2-deoxy-D-ribose for stimulation of wound healing. Journal of Biomaterials Applications, 38(2), 264-279.

ABSTRACT:
Developing multifunctional wound dressings capable of inducing rapid angiogenesis and with antibacterial activity would be attractive for diabetic and superficial wound healing. Hydrogels delivered from tubes have several desirable features -they are easy to apply, keep the wound moist, reduce the entry of microorganisms and avoid the need for painful dressing removal. Previously we reported that 2 deoxy-D-ribose (2dDR) delivered from a variety of dressings is capable of promoting wound healing by stimulating angiogenesis. Alginate hydrogels are an ideal vehicle to deliver a bioactive agent capable of promoting wound healing. In this study we developed and evaluated a tube hydrogel capable of delivering 2dDR with the aim of achieving a

stable, convenient to administer and biologically effective wound treatment. Further, we included the stabilizer 2-phenoxy ethanol which provided antimicrobial activity. We synthesized hydrogels by the Green method, using simple mixing of sodium alginate, propylene glycol, 2-phenoxy ethanol and 2dDR in water. FTIR (Fourier transformation infrared spectroscopy) analysis confirmed an absence of undesirable chemical changes in the gel components, and SEM images of the freeze-dried gels showed porous structures. When 2dDR alginate gel (2dDR-SA hydrogel) was placed in PBS at 37°C, almost 92% of 2dDR was released within 7 days. When tested on cultured cells, 2dDR-SA hydrogels did not inhibit metabolic activity or proliferation, achieving up to 90 and 98% of control respectively over 7 days. 2dDR-SA hydrogel also showed anti-bacterial activity against *E. coli, Pseudomonas aeruginosa, Staphylococcus aureus,* and *MRSA* which was attributable to the stabilizer 2-phenoxy ethanol in the hydrogel. Stimulation of angiogenesis in the chorioallantoic membrane assay by 2dDR-SA hydrogel was found to be significant compared to the blank-SA. Wound healing potential was studied in full-thickness wounds in rats where acceleration of wound healing was seen. H&E staining of the wound tissue showed an enhanced number of blood vessels and re-epithelization, and a reduced number of inflammatory cells in 2dDR-SA treated animals compared to blank-hydrogels while Masson's trichrome staining showed increased collagen deposition. In summary we describe a convenient to apply hydrogel which has promise for use in a range of superficial skin wounds including applications in chronic wound care.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/08853282231191218

6. Rafi, R., Zulfiqar, S., Asad, M., Zeeshan, R., Zehra, M., Khalid, H., ... & Yar, M. (2023). Smart wound dressings based on carbon doped copper nanoparticles for selective bacterial detection and eradication for efficient wound healing application. Materials Today Communications, 35, 105914.

ABSTRACT:

Bacterial infections are considered a major threat worldwide due to the fast emergence of antimicrobial resistance. Real-time monitoring and on time treatment of pathogens is a scientific as well as a practical challenge. The aim of the current research was the development of electrospun wound dressings with potent biocompatible, angiogenic, and antimicrobial action. Antibacterial electrospun polyurethane fibres containing carbon doped copper nanoparticles (C/Cu NPs) were fabricated by electrospinning method and characterized by microscopic and spectroscopic measurements such as scanning electron microscopy, Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction analysis and contact angle measurements. Antibacterial activity of the C/Cu and C/Cu NPs containing polyurethane fibers was evaluated with bacterial strains *Staphylococcus aureus* and *Escherichia coli* and enhanced antibacterial activity was shown by C/Cu NPs and fibers containing C/Cu NPs. *In vitro* cell culture results clearly exhibited these nanoparticles would be helpful in proliferation and migration of fibroblast cells. Results of the wound healing study showed that PU/0.5% NP patches could effectively improve the healing of wounds. The angiogenic potential of the scaffolds was investigated by chorionic allantoic membrane (CAM) assay. Hence, the results

obtained suggest that the fabricated nanofibers are the potential candidate to be used as antibacterial wound dressing for wound healing application.

Web URL: https://www.sciencedirect.com/science/article/pii/S2352492823006050

7. Nasrullah, A., Zahid, M., Ali, A., Ahmad, M. N., Mujahid, A., Hussain, T., ... & Afzal, A. (2023). Ag-ZnS Embedded Polymeric Receptors for the Recognition of Human Serum Albumin. Chemosensors, 11(4), 240.

ABSTRACT:
The detection of human serum albumin (HSA) is of significant clinical importance in disease diagnoses. In this work, polymer-based synthetic receptors are designed by incorporating Ag-ZnS microspheres in molecularly imprinted poly(methacrylic acid-co-ethylene glycol dimethacrylate) (MIPs) for the gravimetric detection of HSA. Among different compositions of Ag-ZnS@MIPs, MIPs having methacrylic acid and ethylene glycol dimethacrylate volume ratio of 3:2 exhibit enhanced HSA sensitivity in the concentration range of 5–200 ng/mL. A remarkably low threshold limit of detection (LOD = 0.364 ng/mL) is achieved with quartz crystal microbalance (QCM) based gravimetric sensors. Furthermore, the Ag-ZnS@MIPs/QCM sensors show high selectivity for HSA compared to other proteins, e.g., bovine serum albumin (BSA), glycoprotein, ribonuclease, and lysozyme. Hence, the gravimetric quantification of HSA realizes a highly sensitive, selective, and label-free detection mechanism with a limit of quantification down to 1.1 ng/mL.

Web URL: https://www.mdpi.com/2227-9040/11/4/240

8. Younas, M., Yar, M., AlMohamadi, H., Mahmood, T., Ayub, K., Khan, A. L., ... & Gilani, M. A. (2024). A rational design of covalent organic framework supported single atom catalysts for hydrogen evolution reaction: a DFT study. International Journal of Hydrogen Energy, 51, 758-773.

ABSTRACT:
Excessive consumption of fossil fuels and CO_2 emissions exacerbate global environmental concerns. Unfortunately, fossil fuel reserves are dwindling and fossil fuel energy is unsustainable, non-renewable, and costly. Due to these concerns, there is an imperative demand for eco-friendly energy conversion electrochemical systems. Hydrogen (H_2) is ubiquitously regarded as a fossil fuel substitute and a potential sustainable energy source. Water electrolysis powered by renewable resources is being considered as a sustainable approach to produce H_2. To cater the need, electrocatalysts with non-precious single metal atoms supported on a covalent organic framework (TM@COF SACs) have been proposed for HER. Single atoms of Co, Ni, Cu, and Zn were introduced onto the COF substrate. The thermodynamic stability, HOMO, LUMO energies, HOMO-LUMO energy gaps, DOS spectra, and change in the Gibbs

free energy of adsorbed atomic hydrogen (ΔG_{H*}) on the catalyst's surface are used to evaluate the catalytic performance of designed complexes for HER. Among all the considered complexes, Zn@COF demonstrated the highest potential to act as a single atom catalyst, with an E_{int} value of −0.11 eV. Density functional theory (DFT) findings suggest that single Zn atom doped on the surface of the covalent organic framework with ΔG_{H*} value of −0.88 eV has a substantial effect on the performance of the HER. This research opens up new possibilities for the advancement and utilization of highly efficient, stable, and cost-effective single-atom catalysts for HER, thereby laying the foundation for future developments in this field.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0360319923034559**

9. Nisar, A., Tabassum, S., Ayub, K., Mahmood, T., AlMohamadi, H., Khan, A. L., ... & Gilani, M. A. (2023). Photoswitchable nonlinear optical properties of azobenzene-based supramolecular complexes: insights from density functional theory. ***Physical Chemistry Chemical Physics*****,** ***25*****(30), 20430-20450**.

ABSTRACT:

Density functional theory (DFT) calculations were performed for a series of supramolecular assemblies containing azobenzene (Azo-X where X = I, Br and H) and alkoxystilbazole subunits to evaluate their electronic, linear and nonlinear optical properties. These assemblies are derivatives of azobenzene, obtained by the substitution of electron-withdrawing and electron-donating groups onto the molecular skeleton. The interaction energies (E_{int}) of all the designed supramolecular complexes (**IA–IF**, **IIA–IIF** and **IIIA–IIIF**) range from −1.0 kcal mol^{-1} to −7.7 kcal mol^{-1}. The electronic properties of these hydrogen/halogen bond driven supramolecular assemblies such as vertical ionization energies (VIE), HOMO–LUMO energy gap ($G_{H–L}$), excitation energies, density of states (DOS) and natural population (NPA) analyses were also computed. The non-covalent interaction index (NCI) and quantum theory of atoms in molecules (QTAIM) analyses were also performed to validate the nature of inter- and intra-molecular interactions in these complexes. A substantial enhancement in the first hyperpolarizability (β_0) values of the designed supramolecular complexes was observed, which is driven by the charge transfer from the pyridyl moiety of alkoxystilbazole to Azo-X. The highest β_0 value of 1.3×10^4 au was observed for the supramolecular complex of *p*-nitro substituted azobenzene with alkoxystilbazole (**ID** complex). Moreover, the results show that the substitution of electron-withdrawing groups on Azo-X can also bring larger β_0 values for such complexes. It was confirmed on a purely theoretical basis that both the types of noncovalent interactions present and the substituent group incorporated influence the nonlinear optical (NLO) response of the systems. Furthermore, the β_0 values of the *E* (*trans*) and *Z* (*cis*) forms were compared to demonstrate the two-way photoinduced switching mechanism.

Web URL: **https://pubs.rsc.org/en/content/articlelanding/2023/cp/d3cp01498c/unauth**

10. Fazal, M. W., Zafar, F., Asad, M., Mohammad H. Al Sulami, F., Khalid, H., Abdelwahab, A. A., ... & Shenashen, M. A. (2023). Zn and Co loaded porous C decorated

electrospun nanofibers as efficient oxygen evolution reaction for water splitting. ACS Applied Energy Materials, 6(5), 2739-2746.

ABSTRACT:
Developing a clean and efficient noble metal free electrocatalyst for oxygen evolution reaction (OER) is urgently needed to accelerate water splitting green energy conversion systems. Herein, we reported the fabrication of a noble metal-free electrocatalyst based on Zn and Co loaded porous C decorated cellulose acetate-polyaniline (ZnCo-C/CA-PANI) electrospun nanofibers at the surface of nickel foam (NF). The smooth coating of CA-PANI electrospun nanofibers at the surface of NF helps in exposing the maximum fraction of ZnCo-C based electrocatalyst and uniform flow of ions at the entire surface, thus resulting in high OH^- adsorption capability. The designed ZnCo-C/CA-PANI@NF electrode acts as an efficient electrocatalyst for oxygen evolution reaction (OER) in an alkaline medium and offers a lower onset potential (1.34 V vs RHE), a small Tafel slope of 42 mV/dec, and high stability. These results suggest a concept of exploring more such noble metal free hybrid materials that could induce the efficient electrocatalytic water splitting for sustainable energy conversion.

Web URL:
https://pubs.acs.org/doi/full/10.1021/acsaem.2c03439?casa_token=rxgVkhloYaIAAAAA%3AZm8y4dx2cQl4mZrtOD5E9KK9xajCxYm5SWZMrFW4mpkDO2lovv22LXUdJs5dImAwVlHR3hvRWXO3wNs

11. Shoukat, N., Anzar, S., Asad, M., Al-Sulami, A. I., Khalid, H., Choudhary, A. A., ... & Akhtar, N. (2023). Fabrication of CuO–NiO wrapped cellulose acetate/polyaniline electrospun nanofibers for sensitive monitoring of bisphenol-A. ACS Sustainable Chemistry & Engineering, 11(11), 4299-4307.

ABSTRACT:
Monitoring endocrine-disrupting chemicals such as bisphenol-A (BPA) is of great concern because its exposure may lead to reproductive problems, neurotoxicity, mutagenicity, and even carcinogenicity. Herein, we reported the fabrication of an efficient electrochemical sensor based on CuO–NiO wrapped cellulose acetate/polyaniline electrospun nanofibers at a Ni foam (CuO–NiO/CA–PANI@NF) electrode for the sensitive and selective monitoring of BPA. CA–PANI-based electrospun nanofibers were selected because of their improved electrical conductivity and charge density, high binding affinity toward BPA via alternative amine and imine groups, and low cost, thus paving the way for the smooth and uniform flow of ions. However, CuO–NiO-based nanoparticles offer more exposed catalytic active species such as NiOOH/CuOOH for the fast electrocatalytic oxidation of BPA. Thus, the synergistic effect of CuO–NiO nanoparticles with electrospun nanofibers leads to high sensitivity (0.00172 μA/nM/cm^2) with a low limit of detection (0.6 nM), a wide linear range (2–100 nM), and high selectivity, even in the presence of interferences, including Co^{2+}, Cd^{2+}, Na^+ Pb^{2+}, Ni^{2+}, Cd^{2+}, Ca^{2+}, Fe^{3+}, NO_3^{2-}, SO_4^{2-}, Cr^{6+}, Br^-, Mg^{2+}, Zn^{2+}, and Ba^{2+} and molecules such as bisphenol-B, bisphenol-F, and phenol. The designed electrode was successfully applied to monitor BPA from plastic bottled water with high precision, thus suggesting the reliability of our designed system

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https://pubs.acs.org/doi/full/10.1021/acssuschemeng.2c04482?casa_token=TGzaDzuS1XYAAAAA%3A8rgSBKy8i0SCmFJv9D2Undz1d1wzvcPEcKILvQdEh_WciqvvmQBFNhI-cZJDsyMjfAdsFm8jN_PbPnc

12. Shah, A. T., Zahoor, M., Muhammad, N., Kamutzki, F., Schmidt, J., & Görke, O. (2023). Rapid wet chemical synthesis of bioactive glass with high yield by probe sonication. Journal of Materials Chemistry B, 11(20), 4416-4427.

ABSTRACT:
Bioactive glasses (BGs) are inorganic biomaterials which possess favourable properties for bone repair and regeneration. The biological properties of the BGs depend on their physical features. This manuscript describes a simple methodology for rapid synthesis of BG nanoparticles (NPs) with tailored physical properties using ultrasonic disruption produced by an ultrasonic probe. The ultrasonic probe generates stable and transient cavitation which increases the mass transfer and accelerates the chemical reaction. This approach is relatively green as it evades the use of the drastic acidic conditions required for hydrolysis. The prepared BG NPs were characterized by Fourier transform infra-red (FTIR) spectroscopy, Raman spectroscopy, scanning electron microscope-energy dispersive X-ray spectroscopy (SEM-EDX), transmission electron microscopy (TEM), X-ray diffraction (XRD), particle size analysis (PSA), nitrogen adsorption/desorption and BET surface area analysis, X-ray photoelectron spectroscopy (XPS), inductively coupled plasma-optical emission spectrometry (ICP-OES), and *in situ* high temperature synchrotron XRD. The effects of ultrasonic irradiation time, and amplitude on the surface properties were investigated and the results confirmed that both parameters, especially amplitude, have significant effects on the physical properties of the prepared BG NPs. The XPS results showed that both, amplitude and time have a pronounced effect on the bridging and non-bridging oxygen atoms bonded to the Si centre in the BG samples, which play an important role in the bioactivity of the BG NPs. The *in situ* high temperature XRD patterns indicated a gradual phase transformation for the BG samples synthesized at different ultrasonic irradiation times and amplitudes. The TEM images showed that uniform nano-sized BG particles were obtained at 50% amplitude in only 10 minutes. A bimodal particle size distribution was observed with an increasing reaction time, up to 30 minutes, due to an increase in the formation of vortices at the interface where nucleation starts. All the prepared samples exhibited a glassy structure with the composition $70SiO_2 : 25CaO : 5P_2O_5$ and were highly bioactive. The proposed method would give a quick route for the synthesis of bioactive glasses and other ceramics with controlled physical properties.

Web URL: https://pubs.rsc.org/en/content/articlelanding/2023/tb/d2tb02385g/unauth

13. Yan, S., Ding, N., Yao, X., Song, J., He, W., Rehman, F., & Guo, J. (2023). Effects of erythromycin and roxithromycin on river periphyton: Structure, functions and metabolic pathways. Chemosphere, 316, 137793.

ABSTRACT:

Macrolides have been frequently detected in the surface waters worldwide, posing a threat to the aquatic microbes. Several studies have evaluated the ecotoxicological effects of macrolides on single algal and bacterial strains. However, without considering the species interaction in the aquatic microbial community, these results cannot be extrapolated to the field. Thus, the present study aimed to evaluate the effects of two macrolides (erythromycin and roxithromycin) on the structure, photosynthetic process, carbon utilization capacity, and the antibiotic metabolic pathways in river periphyton. The colonized periphyton was exposed to the graded concentration (0 μg/L (control), 0.5 μg/L (low), 5 μg/L (medium), 50 μg/L (high)) of ERY and ROX, respectively, for 7 days. Herein, high levels of ERY and ROX altered the community composition by reducing the relative abundance of *Chlorophyta* in the eukaryotic community. Also, the Shannon and Simpson diversity indexes of prokaryotes were reduced, although similar effects were seldomly detected in the low and medium groups. In contrast to the unchanged carbon utilization capacity, the PSII reaction center involved in the periphytic photosynthesis was significantly inhibited by macrolides at high levels. In addition, both antibiotics had been degraded by periphyton, with the removal rate of 51.63–66.87% and 41.85–48.27% for ERY and ROX, respectively, wherein the side chain and ring cleavage were the main degradation pathways. Overall, this study provides an insight into the structural and functional toxicity and degradation processes of macrolides in river periphyton.

Web URL: https://www.sciencedirect.com/science/article/pii/S0045653523000590

14. Rehman, F., Khan, A. J., Alobaid, H. M., Gilani, M. A., Safi, S. Z., Muhammad, N., ... & Emran, T. B. (2023). Surface engineered mesoporous silica carriers for the controlled delivery of anticancer drug 5-fluorouracil: Computational approach for the drug-carrier interactions using density functional theory. Frontiers in Pharmacology, 14, 1146562.

ABSTRACT:

Introduction: Drug delivery systems are the topmost priority to increase drug safety and efficacy. In this study, hybrid porous silicates SBA-15 and its derivatives SBA@N and SBA@3N were synthesized and loaded with an anticancer drug, 5-fluorouracil. The drug release was studied in a simulated physiological environment.

Method: These materials were characterized for their textural and physio-chemical properties by scanning electron microscopy (SEM), nuclear magnetic resonance (NMR), Fourier transform infrared spectroscopy (FTIR), small-angle X-ray diffraction (SAX), and nitrogen adsorption/desorption techniques. The surface electrostatics of the materials was measured by zeta potential.

Results: The drug loading efficiency of the prepared hybrid materials was about 10%. *In vitro* drug release profiles were obtained in simulated fluids. Slow drug release kinetics was observed for SBA@3N, which released 7.5% of the entrapped drug in simulated intestinal fluid (SIF, pH 7.2) and 33% in simulated body fluid (SBF, pH 7.2) for 72 h. The material SBA@N presented an initial burst release of 13% in simulated intestinal fluid and 32.6% in simulated gastric fluid (SGF, pH 1.2), while about 70% of the drug was released within the next 72 h. Density functional theory (DFT) calculations have also supported the slow drug release from the SBA@3N material. The release mechanism of the drug from the prepared carriers was studied by first-order, second-order, Korsmeyer–Peppas, Hixson–Crowell, and Higuchi kinetic models. The

drug release from these carriers follows Fickian diffusion and zero-order kinetics in SGF and SBF, whereas first-order, non-Fickian diffusion, and case-II transport were observed in SIF.
Discussion: Based on these findings, the proposed synthesized hybrid materials may be suggested as a potential drug delivery system for anti-cancer drugs such as 5-fluorouracil.

Web URL:
https://www.frontiersin.org/journals/pharmacology/articles/10.3389/fphar.2023.1146562/full

15. us Sama, Z., Khan, A. J., Rehman, F., Gul, S., Safi, S. Z., Imran, M., & ud Din, Z. (2023). In silico approach to explore anti-chikungunya potential of Schiff's bases with benzene and pyrimidine moieties. Chemical Papers, 77(8), 4489-4500.

ABSTRACT:
In this study, hydrazone derivatives (D1–D3) were synthesized aiming to evaluate its anti-chikungunya activity using in silico approach. Density functional theory calculation showed that the electronic density lies on the central aromatic rings of these molecules. Best confirmer, with minimum energy of these hydrazones, was selected for docking studies against the protein (PDB: ID 3gpg) to discover the anti-chikungunya potential. Significant interactions were observed between these compounds and with the amino acids of the active site of protein 2vbc. Based on the computational approach, it could be suggested that the proposed compounds have strong anti-chikungunya actives and could be further investigated as potential anti-chikungunya drug.

Web URL: https://link.springer.com/article/10.1007/s11696-023-02800-9

16. Ghafoor, M., Khan, Z. U., Nawaz, M. H., Akhtar, N., Rahim, A., & Riaz, S. (2023). In-situ synthesized ZIF-67 graphene oxide (ZIF-67/GO) nanocomposite for efficient individual and simultaneous detection of heavy metal ions. Environmental Monitoring and Assessment, 195(3), 423.

ABSTRACT:
Heavy metals are ubiquitous in water bodies as a result of anthropogenic activities and over time they accumulate in body thus posing serious health problems. Therefore, it is essential to improve sensing performance, for determination of heavy metal ions (HMIs), of electrochemical sensors. In this work, cobalt-derived MOF (ZIF-67) was in-situ synthesized and incorporated onto the surface of graphene oxide (GO) by simple sonication method. The prepared material (ZIF-67/GO) was characterized by FTIR, XRD, SEM, and Raman spectroscopy. Afterwards, a sensing platform was made by drop-casting synthesized composite onto glassy carbon electrode for individual and simultaneous detection of heavy metal ions pollutants (Hg^{2+}, Zn^{2+}, Pb^{2+}, and Cr^{3+}) with estimated detection limits of 2 nM, 1 nM, 5 nM, and 0.6 nM, respectively, when determined simultaneously, that are below the permissible limit by World Health Organization. To the best of our knowledge, this is first report of HMIs detection by ZIF-67 incorporated GO sensor which can successfully determine the Hg^{+2}, Zn^{+2}, Pb^{+2}, and Cr^{+3} ions simultaneously with lower detection limits.

Web URL: https://link.springer.com/article/10.1007/s10661-023-10966-8

17. Amara, U., Mahmood, K., Khan, M., & Nawaz, M. H. (2023). Polypyrrole enwrapped binary metal oxides nanostructures for in-vitro Dopamine detection from lacrimal fluid. Microchemical Journal, 185, 108254.

ABSTRACT:
Dopamine (DA) disorder has been associated in pathogenesis of many neuronal dysfunction. So, DA homeostasis is the thumbprint of enduring neuronal health and physiological condition. However, the development of molecular probes that allow in vitro screening of DA with spatiotemporal resolution is a great challenge. For this purpose, we report a synthesis, characterization and application of lanthanum oxide modified iron oxide nanoparticles enwrapped polypyrrole interface (La_2O_3@Fe_2O_3/PPy). This newly integrated material has been characterized via Raman spectroscopy, Scanning electron microscopy (SEM), Zeta Potential, X-ray diffraction spectroscopy (XRD) and Atomic force microscopy (AFM). The Fe_2O_3 created passage for electron transportation owing to presence of redox active sites, La_2O_3 introduction induced massive defects for analyte adsorption and PPy provided stability with enhanced electron shuttling. These synergistic properties eventually amplified the transduction signals leading to the higher electrocatalytic activity for DA oxidation. The designed La_2O_3@Fe_2O_3/PPy transducing interface accomplished selective DA sensing and a detection limit was found to be 1.2 nM in the linear bounds of 100 μM to 3.5 mM. In addition, the interface was effectively utilized to detect dopamine from the lacrimal fluid with decent recoveries. We antedate that this design will pave the ways for the in vitro analysis of DA from real samples with desired selectivity and sensitivity.

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18. Amara, U., Mahmood, K., Khan, M., & Nawaz, M. H. (2023). Polypyrrole enwrapped binary metal oxides nanostructures for in-vitro Dopamine detection from lacrimal fluid. Microchemical Journal, 185, 108254.

ABSTRACT:
Dopamine (DA) disorder has been associated in pathogenesis of many neuronal dysfunction. So, DA homeostasis is the thumbprint of enduring neuronal health and physiological condition. However, the development of molecular probes that allow in vitro screening of DA with spatiotemporal resolution is a great challenge. For this purpose, we report a synthesis, characterization and application of lanthanum oxide modified iron oxide nanoparticles enwrapped polypyrrole interface (La_2O_3@Fe_2O_3/PPy). This newly integrated material has been characterized via Raman spectroscopy, Scanning electron microscopy (SEM), Zeta Potential, X-ray diffraction spectroscopy (XRD) and Atomic force microscopy (AFM). The Fe_2O_3 created passage for electron transportation owing to presence of redox active sites, La_2O_3 introduction induced massive defects for analyte adsorption and PPy provided stability with enhanced electron shuttling. These synergistic properties eventually amplified the transduction signals

leading to the higher electrocatalytic activity for DA oxidation. The designed La_2O_3@Fe_2O_3/PPy transducing interface accomplished selective DA sensing and a detection limit was found to be 1.2 nM in the linear bounds of 100 µM to 3.5 mM. In addition, the interface was effectively utilized to detect dopamine from the lacrimal fluid with decent recoveries. We antedate that this design will pave the ways for the in vitro analysis of DA from real samples with desired selectivity and sensitivity.

Web URL: https://www.sciencedirect.com/science/article/pii/S0026265X22010827

19. Nawaz, M. A. H., Fazal, M. W., Akhtar, N., Nawaz, M. H., Hayat, A., & Yu, C. (2022). Multifunctional smart ZnSe-nanostructure-based fluorescent aptasensor for the detection of ochratoxin A. Biosensors, 12(10), 844.

ABSTRACT:

Herein, we present a comprehensive investigation of rationally designed zinc selenide (ZnSe) nanostructures to achieve highly negatively charged ZnSe nanostructures. A Microwave-assisted hydrothermal synthesis method was used to synthesize three types of ZnSe nanostructures, i.e., nanorods, µ-spheres and nanoclusters, as characterized by a zeta potential analyzer, X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy and BET, which were labeled as type A, B and C. Three different solvents were used for the synthesis of type A, B and C ZnSe nanostructures, keeping other synthesis conditions such as temperature, pressure and precursors ratio constant. Based on two heating time intervals, 6 and 9 h, types A, B and C were further divided into types A6, A9, B6, B9, C6 and C9. ZnSe nanostructures were further evaluated based on their fluorescent quenching efficiency. The maximum fluorescence quenching effect was exhibited by the ZnSe-B6 type, which can be attributed to its highly negative surface charge that favored its strong interaction with cationic dye Rhodamine B (Rh-B). Further, the optimized ZnSe-B6 was used to fabricate an aptasensor for the detection of a food-based toxin, ochratoxin-A (OTA). The developed aptasensor exhibited a limit of detection of 0.07 ng/L with a wide linear range of 0.1 to 200 ng/L

Web URL: https://www.mdpi.com/2079-6374/12/10/844

20. Ramzan, A., Mehmood, A., Ashfaq, R., Andleeb, A., Butt, H., Zulfiqar, S., ... & Riazuddin, S. (2023). Zinc oxide loaded chitosan-elastin-sodium alginate nanocomposite gel using freeze gelation for enhanced adipose stem cell proliferation and antibacterial properties. International Journal of Biological Macromolecules, 233, 123519.

ABSTRACT:

Hydrogels have been the material of choice for regenerative medicine applications due to their biocompatibility that can facilitate cellular attachment and proliferation. The present study aimed at constructing a porous hydrogel composite scaffold (chitosan, sodium alginate and elastin) for the repair of chronic skin wounds. Chitosan-based hydrogel incorporating varying concentrations of zinc oxide nanoparticles i.e. ZnO-NPs (0, 0.001, 0.01, 0.1 and 1 % *w/w*) as the antimicrobial agent tested against *Escherichia coli* (*E.coli*) and Staphylococcus aureus (*S. aureus*) exhibited good antibacterial activities. ZnO-NPs were characterized by UV visible spectroscopy, Scanning

electron microscopy (SEM) analysis, Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) analysis. Fabricated gels were characterized by SEM analysis, FTIR, XRD, swelling ratio, degradation behavior and controlled release kinetics of ZnO-NPs. In vitro cytocompatibility of the composite was investigated using human adipose stem cells (ADSCs) by MTT and lactate dehydrogenase (LDH) assay, further assessed by SEM analysis and PKH26 staining. The SEM and XRD analysis confirmed the successful loading of ZnO-NPs into these scaffolds. Fluorescence PKH26 stained images and SEM analysis of ADSCs seeded scaffolds revealed biocompatible nature. The findings suggested that the developed composite gels have potential clinically for tissue engineering and chronic wound treatment.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813023004129

21. Bano, R., Ayub, K., Mahmood, T., Arshad, M., Sharif, A., Tabassum, S., & Gilani, M. A. (2023). Diamondoid as potential nonlinear optical material by superalkali doping: a first principles study. Diamond and Related Materials, 135, 109826.

ABSTRACT:

Adamantane ($C_{10}H_{16}$), the smallest diamondoid molecule, has sparked considerable scientific interest due to its symmetric, single cage-shaped structure. In the current work, the geometric, electronic, and nonlinear optical responses of Li_3O, Na_3O and K_3O clusters doped adamantanes have been investigated via DFT simulations. The calculated values of interaction energies (−5.50 to −6.91 kcal/mol) and vertical ionization energies (3.01–3.56 eV) reflected that the designed M_3O-Ada complexes are thermodynamically and chemically stable. Charge transfer is probed through natural population analysis and the highest charge transfer (0.038 |e|) is observed for K_3O-Ada complex. The electride nature of M_3O-Ada complexes is confirmed through their electron density distribution and their energy gaps (2.19–3.06 eV) are reduced significantly. Interestingly, the absorption maxima (1387–1629 nm) of M_3O-Ada electrides fall in the near infrared region. The highest first and second hyperpolarizability values of 5.9×10^5 au and 2.6×10^8 au are observed for K_3O-Ada electride. The maximum hyper-Rayleigh scattering and second harmonic generation values of 1.3×10^7 au and 6.5×10^6 au are obtained at 1907 nm whereas the electro-optical Pockel's effect (6.5×10^6 au) is maximum at 1064 nm. Moreover, the dynamic second hyperpolarizability co-efficients (EOKE, EFISHG) are also computed at varying wavelengths. The M_3O-Ada electrides exhibit the maximum nonlinear refractive index n_2 of 1.9×10^{-7} cm^2 W^{-1} at 1064 nm. This study will pave the way to the designing of stable superalkali doped diamondoids with enhanced NLO response.

Web URL: https://www.sciencedirect.com/science/article/pii/S0925963523001516

***22.* Ahmad, A., Mansor, N., Mahmood, H., Sharif, F., Safdar, R., & Moniruzzaman, M. (2023). Evaluation thermal degradation kinetics of ionic liquid assisted polyetheretherketone-multiwalled carbon nanotubes composites. *Journal of Applied Polymer Science*, *140*(12), e53647.**

ABSTRACT:

The incorporation of multiwalled carbon nanotubes (MWCNT) into polyetheretherketone (PEEK) composites has emerged as a promising strategy for enhancing the thermomechanical characteristics of PEEK composite materials. This study investigates the thermal behavior and kinetics prediction of PEEK/MWCNT composites comprising different ionic liquids (ILs), namely 1-butyl-3-methylimidazolium hydrogen sulfate ([BMIM]HSO_4), 1-butyl-3-methylimidazolium acetate ([BMIM]Ac), 1-ethyl-3-methylimidazolium acetate ([EMIM]Ac) and 1-ethyl-3-methylimidazolium hydrogen sulfate ([EMIM]HSO_4). Three non-isothermal methods Coats-Redfern, Broido, and Horowitz-Metzger, were employed to model the thermal decomposition profiles of fabricated composites to calculate the activation energy. The highest decomposition temperature (580°C) was obtained for [BMIM]HSO_4-based PEEK/MWCNT composites. Moreover, a 3%–8% increase in the activation energy was obtained compared to PEEK/MWCNT manufactured without ILs. The Coats-Redfern model was superior to Broido and Horowitz-Metzger models in modeling the thermal degradation of developed composites, as evidenced from the higher value of the coefficient of determination ($R^2 \geq 0.9899$). By determining the Root Mean Square Error (RMSE) and R^2 for the thermal degradation kinetics data, the artificial neural network (ANN) model was employed. The ANN model accurately predicted the mass loss curves, exhibiting $R^2 \geq 0.9815$ for the designed model. These findings can assist in establishing an IL-assisted benign approach for PEEK/MWCNT/IL composites with superior thermal characteristics.

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/app.53647

23. Samie, M., Khan, A. F., Rahman, S. U., Iqbal, H., Yameen, M. A., Chaudhry, A. A., ... & Hardy, J. G. (2023). Drug/bioactive eluting chitosan composite foams for osteochondral tissue engineering. International Journal of Biological Macromolecules, 229, 561-574.

ABSTRACT:

Joint defects associated with a variety of etiologies often extend deep into the subchondral bone leading to functional impairment and joint immobility, and it is a very challenging task to regenerate the bone-cartilage interface offering significant opportunities for biomaterial-based interventions to improve the quality of life of patients. Herein drug-/bioactive-loaded porous tissue scaffolds incorporating nano-hydroxyapatite (nHAp), chitosan (CS) and either hydroxypropyl methylcellulose (HPMC) or Bombyx mori silk fibroin (SF) are fabricated through freeze drying method as subchondral bone substitute. A combination of spectroscopy and microscopy (Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive X-ray (EDX), and X-ray fluorescence (XRF) were used to analyze the structure of the porous biomaterials. The compressive mechanical properties of these scaffolds are biomimetic of cancellous bone tissues and capable of releasing drugs/bioactives (exemplified with triamcinolone acetonide, TA, or transforming growth factor-β1, TGF-β1, respectively) over a period of days. Mouse preosteoblast MC3T3-E1 cells were observed to adhere and proliferate on the tissue scaffolds as confirmed by the cell attachment, live-dead assay and alamarBlue™ assay. Interestingly, RT-qPCR analysis showed that the TA downregulated inflammatory biomarkers and upregulated the bone-specific biomarkers, suggesting such tissue scaffolds have long-term potential for clinical application.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813022032160

24. Assiri, M. A., Hanif, S., Junaid, H. M., Hamad, A., Irshad, H., Yar, M., ... & Shahzad, S. A. (2023). AIEE active fluorophores for the sensitive detection of iron ions: An advanced approach towards optical and theoretical investigation. Journal of Photochemistry and Photobiology A: Chemistry, 438, 114514.

ABSTRACT:
Iron is an essential microelement and the most abundant transition metal in humans that catalyzes different crucial metabolisms. It also has broader industrial applications as a precursor for the manufacturing of different domestic products. However, its excess in the biological and environmental matrixes induce adverse health effects. Considering the significant role of the iron in numerous biological processes and environmental safety threats, immediate sensing of iron in a complex system is inevitably pivotal. In the pursuit of these concerns, two efficient solvatochromic and AIEE active TPA based sensors **TPA 1** and **TPA 2** were critically designed and synthesized for the development of efficient sensing materials. The proposed sensors **TPA 1** and **TPA 2** were exploited as an easy-to-apply platform for the sensitive and selective optical tracing of the iron (Fe (II)) in aqueous media (H_2O/THF; 4:1, v/v) through sensor–metal chelation induced fluorescence quenching (CHEQ) mechanism with LOD down to 15 and 19 nM, respectively. The optical investigations were validated through ^1H NMR titration, extensive theoretical studies, and Jobs plot experiment. Further, AIEEgens were advantageously utilized to establish the ready-to-use and hand-held fluorescent kits for the solid state Fe (II) trailing. The spike-recovery experiments were executed to quantify Fe (II) in wheat flour and real water samples. Besides, the practical applicability potential of the designed sensors was explored by executing MTT assay and monitoring of the Fe (II) in blood serum samples. Additionally, a logic circuit was rationally fabricated for the digital on-field sensing of Fe (II). To the best of our knowledge, these are the first TPA based compounds with fabulous structural simplicity, and startling practical applicability as sensitive iron sensors.

Web URL: https://www.sciencedirect.com/science/article/pii/S1010603022007377

25. Ali, Z., Ullah, R., Tuzen, M., Ullah, S., Rahim, A., & Saleh, T. A. (2023). Colorimetric sensing of heavy metals on metal doped metal oxide nanocomposites: A review. Trends in Environmental Analytical Chemistry, 37, e00187.

ABSTRACT:
Heavy metal ion-containing pollution has drawn a lot of attention. It presents thoughtful risks to the human situation and environmental system. Nanotechnologies can control, create, and measure objects on a molecular and atomic size between 1 and 100 nm. Their surface area to volume ratio is high. These are the most practical and are to blame for the easy accessibility, particularly for environmental cleanup. The nanocomposites have proven to offer remarkable qualities as platforms for heavy metal detection sensing. Monitoring the water quality is one of the key concerns of researchers in the modern period. Heavy metal contamination is a significant

issue and poses a risk to ecological preservation. Due to this, several efforts are being made in present to develop sensitive, quick, and selective sensors. Reversibility, high specificity, and sensitivity are three unique and intriguing characteristics of colorimetric sensors that have grown in popularity. The particular features of nanomaterials, such as those based on metal and metal oxide, polymers, and carbon, make them beneficial for cleaning up the environment. We examined the most recent (2010–2022) advancements in metal composites for the treatment of metal ions in contaminated water in this review study.

Web URL: https://www.sciencedirect.com/science/article/pii/S2214158822000344

26. Yousaf, S., Akhtar, T., AlMasoud, N., Ayub, K., Rauf, S., Tariq, M., ... & El-Bahy, Z. M. (2023). Porphyrin-Anhydride Co-Sensitization Strategy for Enhanced Photovoltaic Performance in DSSC: A Combined Experimental and Theoretical Approach. Polyhedron, 246, 116675.

ABSTRACT:

A new covalently linked porphyrin-based anhydride($C_{108}H_{86}N_{10}O_4Zn_2$) named TPP-PMDI-TPP has been successfully synthesized through a simple thermal imidization reaction of electron-donating Zn(5-(4-aminopheny)-10,15,20-triphenylporphyrin(Zn-ATPP) and electron-accepting pyromellitic dianhydride(PMDA) moieties and tested in the of photovoltaic application. TPP-PMDI-TPP was subjected to comprehensive characterization using various analytical techniques, including FT-IR, ^{1}H NMR, UV–visible, PXRD, cyclic voltammetry, and molecular simulation. Fluorescence studies were also employed to characterize TPP-PMDI-TPP. Excellent fluorescence quenching of 95 % was observed in TPP-PMDI-TPP, indicating remarkable electron transfer from porphyrin to pyromellitic dianhydride within TPP-PMDI-TPP. The cyclic voltammetric analysis provided the HOMO and LUMO values of TPP-PMDI-TPP as −6.172 eV and −4.185 eV, respectively. The investigation of the charge-transfer phenomenon in the entitled compound was assessed using FMOs. Results obtained from cyclic voltammetry and computational calculations for HOMO, LUMO, and band gap (E_g) of porphyrin-based anhydride (TPP-PMDI-TPP) are in well concordance, indicating the practicality of the utilized experimental approach. Global reactivity parameters were obtained by using HOMO–LUMO energies of compounds. The photovoltaic measurements of ITO-coated TPP-PMDI-TPP film was performed to check different photovoltaic parameters (V_{OC}, I_{SC}, FF, and η), showing values of about 0.858 V, 8.1794 mA/cm^2, 0.561 and 3.9 % respectively, calculated from current-voltage (I–V) graph. The lower photocurrent and power conversion efficiency in the TPP-PMDI-TPP film is due to the electron withdrawal caused by the dianhydride group, transferring electrons from porphyrin to PMDA. This electron-withdrawing effect leads to imbalanced charge transport, with higher hole mobilities than electron mobilities, resulting in lower efficiency for TPP-PMDI-TPP-based photovoltaic cells.

Web URL: https://www.sciencedirect.com/science/article/pii/S0277538723003972

27. Bokhari, N., Ali, A., Yasmeen, A., Khalid, H., Safi, S. Z., & Sharif, F. (2023). Fabrication of green composite hand knitted silk mesh reinforced with silk hydrogel. International Journal of Biological Macromolecules, 253, 127284.

ABSTRACT:

Soft tissue defects like hernia and post-surgical fistula formation can be resolved with modern biomaterials in the form of meshes without post-operative complications. In the present study hand knitted silk meshes were surface coated with regenerated silk fibroin hydrogel and pure natural extracts. Two phytochemicals (Licorice extract (LE) and Bearberry extract (BE)) and the two honeybee products (royal jelly (RJ) and honey (HE)) were incorporated separately to induce antibacterial, anti-inflammatory, and wound healing ability to the silk hydrogel coated knitted silk meshes. Meshes were dip coated with a blend of 4 % silk hydrogel (w/v) and 5 % extracts. Dried modified meshes were characterized using SEM, DMA, GC–MS and FTIR. Antimicrobial testing, in-vitro cytotoxicity, in-vitro wound healing and Q-RT-PCR were also performed.

SEM analysis concluded that presence of coating reduced the pore size up to 47.7 % whereas, fiber diameter was increased up to 17.9 % as compared to the control. The presence of coating on the mesh improved the mechanical strength/Young's modulus by 1602.8 %, UTS by 451.7 % and reduced the % strain by 51.12 %. Sustained release of extracts from MHRJ (62.9 % up to 72 h) confirmed that it can induce antibacterial activity against surgical infections. Cytocompatibility testing and gene expression results suggest that out of four variables MHRJ presented best cell viability, % wound closure and expression of wound healing marker genes. In-vivo analyses in rat hernia model were carried out using only MHRJ variant, which also confirmed the non- toxic nature and wound healing characteristics of the modified mesh. The improved cell proliferation and activated wound healing in vitro and in vivo suggested that MHRJ could be a valuable candidate to promote cell infiltration and activate soft tissue and hernia repair as a biomedical implant.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813023041818

28. Bukhari, A., Yar, M., Zahra, F., Nazir, A., Iqbal, M., Shah, S. A. A., ... & Ahmad, N. (2023). A novel formulation of triethyl orthoformate mediated durable, smart and antibacterial chitosan cross-linked cellulose fabrics. *International Journal of Biological Macromolecules*, *253*, 126813.

ABSTRACT:

Antibacterial, durable and smart cotton fabrics was developed using chitosan-based formulation. The cellulose was covalently cross-linked with chitosan using TEOF. The antibacterial activity of prepared smart fabrics and CS was studied against *S. aureus* and *E. coli* strains. The FTIR, SEM and XRD were employed to confirm the linkage of CS molecules with cellulose in cotton fabrics. The CS of 160 KDa extracted from shrimp shell showed the optimum antibacterial activity. The prominent asymmetric, symmetric alkyl Csingle bondH peaks of CS were shifted to 2930 and 2845 (cm^{-1}), respectively. Moreover, the shifted peaks at 1590 and 1400 (cm^{-1}) indicate the Csingle bondO stretching and NH_2 bending bands of CS, respectively. This confirm

the existence of new imine functional group that was generated after cross-linking of NH_2 groups of CS. The SEM results showed more uniform morphology of TEOF cross-linked fabrics versus CS coated fabrics, which revealed a promising microbial growth inhibition activity. The TEOF as a cross-linker has been unveiled, showcasing the effectiveness of this innovative crosslinking approach. The fabric treated with cross-linked CS exhibited remarkable antibacterial properties that endured even after undergoing 30 washing cycles. These antibacterial textiles possess substantial commercial potential across a diverse range of industries.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813023037108

29. Hameed, S., Hayat, A., Alghamdi, E. A., Bano, N., Jubeen, F., & Khurramd, A. (2023). A review on recent advances in covalent organic frameworks-based membranes: synthesis, modification, and applications in liquid phase separation. Journal of Science: Advanced Materials and Devices, 100632.

ABSTRACT:

The ever-growing global population and the scarcity of clean water resources are major social challenges. In response, researchers are exploring novel materials for water treatment, with a focus on producing high-quality drinkable water for various uses. Covalent organic frameworks (COFs) are a type of porous organic polymers that possess well-defined pore architectures and are constructed through covalent bonds between organic building blocks. COFs offer considerable potential in the field of membrane separation due to their unique characteristics, such as consistent pore sizes, regular pores, and diverse pore environments. In this review paper, we provide an in-depth evaluation of the recent advancements in the synthesis and modification of COF-based membranes, including the fabrication of hybrid COFs, surface modification, and defect engineering for liquid phase separation. Firstly, we discuss conventional COF processing techniques such as support-assisted, free-standing, and mixed matrix membranes (MMM). Secondly, the reactivity of synthesizing monomers is a critical factor in the development of advanced COF-based membranes. Therefore, we emphasize the nature and reactivity of reacting amine and aldehyde monomers and their significant implications for enhancing the properties and performance of COFs membranes. Finally, we highlight the applications of COF membranes in water treatment, organic solvent nanofiltration, desalination, and heavy metal recovery operations. Our comprehensive review aims to provide an essential guide for researchers in the field of liquid phase separation techniques with an interest in developing unique COF membranes for improved water treatment processes.

Web URL: https://www.sciencedirect.com/science/article/pii/S2468217923001016

30. Farman, H., Khan, M. A., Alamoudi, A. J., Sharif, F., Alshamrani, M., Liaqat, S., ... & Muhammad, N. (2023). Fabrication of polymeric composite GTR membrane from eggshell powder, polylactic acid and polyethylene glycol for periodontal application: in vitro evaluation. Frontiers in Materials, 10, 1234065.

ABSTRACT:

This study aims to fabricate, characterize and evaluate Guided tissue regeneration (GTR) membrane containing eggshell (ES), chlorhexidine (CHX) and polymeric matrix for periodontal application. ES powder ground to size 74 µm was mixed in Polylactic Acid (PLA) and Polyethylene Glycol (70:30 ratios) mixture in 10% and 30% wt to fabricate the membrane and named groups C-10 and C-30. Along with this, 0.25% and 0.5% CHX powder were adsorbed on ES powder and incorporated in PLA and PEG mixture to fabricate drug containing groups C-10CHX and C-30CHX respectively. UTM was used to measure tensile strength, Young's Modulus, and percent elongation of the prepared GTR membrane. Experimental groups containing 10% ES powder (C-10 and C-30) had adequate tensile properties. The percent mass change of the samples was calculated by the change in weight of the samples (W_d) from the weight of samples after immersion in phosphate-buffered saline PBS (W_t). Contact angle measurement showed that all membranes were found to be hydrophilic (contact angle<90). Groups containing the drug CHX (C-10CHX and C-30CHX) had significant disc diffusion antibacterial activity. Cell viability assay was carried out by Alamar Blue Assay using mouse fibroblasts NIH3T3 and pre-osteoblasts that indicated very good biocompatibility of the groups (C, C-10, C-30, and C-10CHX) while experimental group C-30CHX showed slight cytotoxicity (Cell Viability >70%).

Web URL:
https://www.frontiersin.org/journals/materials/articles/10.3389/fmats.2023.1234065/full

31. Badar, R., Zulfiqar, S., Zahid, A. A., Mehmood, N., Zeeshan, R., Nawaz, A., ... & Yar, M. (2023). Thyroxine incorporated commercially available alginate dressings to stimulate angiogenesis for wound healing applications. Journal of Drug Delivery Science and Technology, 89, 105026.

ABSTRACT:

Advanced wound care products had attracted great attention and particularly materials stimulating angiogenesis is one of the major focussed area. The identification of suitable angiogenic agents and then delivery from a well accepted carrier materials, ideally the one being already in clinical use is well adopted approach. Alginate dressings are very well accepted dressings worldwide in clinic and in present work alginate dressings were modified to support angiogenesis by loading thyroxine. To study the affect of concentration of thyroxine, 1 µg/ml, 5 µg/ml and 10 µg/ml thyroxine was loaded into alginate dressings. Any chemical changes in the dressings after loading thyroxine was studied by FTIR analyses and it was found that loading of thyroxine did not produce any chemical change in alginate dressings. The sustained thyroxine release up to 74% was observed in the phosphate buffer pH 7.4 over seven days time. The cytotoxicity study was conducted using fibroblasts cells and all thyroxine concentrations were found to be biocompatible and assisted cells proliferation. Real time PCR was used to evaluate the gene expression of fibroblasts treated with synthesized alginate hydrogels to evaluate the effect of thyroxine on genes involves in angiogenic pathway. To study angiogenic activity chorioallantoic membrane (CAM) assay was performed, it was observed higher number of new junctions, angiogenic potential was shown by 5 µg/ml thyroxine loaded alginate dressings. These results suggested that the thyroxine loaded alginate dressings have very high potential of fast wound healing.

Web URL: https://www.sciencedirect.com/science/article/pii/S177322472300878X

32. Mustafai, A., Hussain, A., Yar, M., Hussain, R., Ayub, K., Imran, M., & Assiri, M. A. (2023). Triquinoxalinylene and benzoquinone based covalent organic framework as robust material for mitigation of environmental pollutants-A theoretical approach. Journal of Molecular Liquids, 391, 123304.

ABSTRACT:

The physisorption of pollutant gases (NH_3, HCN, H_2S and PH_3) on TQBQ-COF has been explored using DFT calculations. The strength and nature of interactions were determined through interaction energy, non-Covalent interactions- Reduced Density Gradient (NCI-RDG) plots, Frontier Molecular Orbital (FMO), Natural bond orbital (NBO), Electron Density Difference (EDD) and Quantum Theory of Atoms In Molecule (QTAIM) analysis. The optimized geometries and interaction energy calculations revealed that the analytes interacted with Oxygen and Nitrogen atoms of TQBQ-COF leading to adsorption energy ranging from −10.66 to −5.85 kcal/mol. The values of recovery time were in agreement to that of interaction energy and decreased with the increase in temperature. The NCI-RDG plots and QTAIM analysis revealed the presence of weak van der Waals forces in all complexes and partial covalent character in H_2S@TQBQ-COF. Charge transfer study (employing NBO and EDD analysis) depicted the transfer of charge from surface to analytes. The study of HOMO-LUMO energy gap in FMO analysis depicted the high sensitivity of TQBQ-COF for H_2S and NH_3 compared to HCN and PH_3 due to significant lowering of HOMO-LUMO energy gap upon the adsorption of H_2S and NH_3 on TQBQ-COF.

Web URL: https://www.sciencedirect.com/science/article/pii/S0167732223021104

33. Buzdar, M., Yaqub, A., Hayat, A., Haq, M. Z. U., Khan, A., & Ajab, H. (2023). Paper based colorimetric sensor using novel green magnetized nanocomposite of pinus for hydrogen peroxide detection in water and milk. Food Bioscience, 55, 103014.

ABSTRACT:

The present work was focused on the Hydrogen peroxide (H_2O_2) detection by designing a portable and sustainable filter paper based sensor based on novel use of green enzyme mimic magnetic nanoparticles of *Pinus* needles (MNP). The nanozymes were synthesized via an easy ecofriendly and cheap route besides characterized by UV–Vis spectroscopy, Scanning Electron Microscope, Fourier transform infrared spectroscopy, Zeta potential, X-ray diffraction and Vibrating Sample Magnetometer etc. The characterization study supported the suitability and optical properties of MNP for sensor fabrication like presence of various functional groups, availability of binding sites, moderate stability, super paramagnetic properties and amorphous structure etc. The coactive effect of *Pinus* needles and magnetic nanoparticles components on sensing platform demonstrated an inherent peroxidase-like activity with enhanced optical response for catalyzing the oxidation of substrate 3,3′,5,5′-tetramethylbenzidine with perceived naked eye reaction. The optimization was carried out with respect to different parameters such as incubation time (15 min), Gel concentration (0.2 mg/mL) and concentration of MNP (2 mg/mL) etc. A good sensitivity was achieved by using color analyzing model at a lower limit of detection

(LOD) 0.007 μM in a relative wide-ranging of 0.01 μM–0.09 μM. The application in biological and samples environmental (tap water and milk) indicated that the proposed paper-based sensor delivers reasonable platforms for simple, sustainable, and quick detection of H_2O_2 with high selectivity.

Web URL: https://www.sciencedirect.com/science/article/pii/S221242922300665X

34. Suhail, F., Batool, M., Anjum, T., Shah, A. T., Tabassum, S., Khan, A. L., ... & Gilani, M. A. (2023). Enhanced CO2 separation performance of polysulfone membranes via incorporation of pyrazole modified MCM-41 mesoporous silica as a nano-filler. Fuel, 350, 128840.

ABSTRACT:

Polymeric membranes are one of the widely used materials of choice for CO_2 capture from major industrial sources. However, the current generation of polymeric materials are unable to keep up with the increasing separation needs of CO_2 from the air (CO_2/N_2) or natural gas (CO_2/CH_4) on an industrial scale due to their so-called permeability-selectivity tradeoff. In an effort to improve the overall gas separation performance of polymeric membranes, mixed matrix membranes (MMMs) have been suggested as a substitute strategy. In this study, Polysulfone (PSf) based MMMs were prepared by incorporating pyrazole modified MCM-41 mesoporous silica (MP) as a nano-filler in the polymer matrix to enhance the gas separation properties of membranes. MCM-41 nano-filler was synthesized and functionalized by post-grafting technique to prepare the MMMs of three different loadings (10, 20, and 30 wt%). All the membranes were characterized for physical, chemical, and thermal analysis. The CO_2 gas separation performance of membranes was assessed, and the results concluded that the MCM-41-based MMMs showed the tradeoff between permeability and selectivity in the case of ideal and mixed gases. This permeability-selectivity trade-off is solved by the MP-based MMMs due to the presence of CO_2-philic functional groups present on the surface of membranes. The PSf-MP membrane with the highest nanofiller loading (30 wt%) showed 79% more permeability than the pure PSf membrane. Additionally, it showed a significant enhancement of 33% and 51% in ideal selectivity for CO_2/CH_4 and CO_2/N_2, respectively, compared to pure PSf membrane. These findings support the lack of membrane faults, the enhanced filler/polymer interface, and the remarkable nano-filler dispersion in the polymer matrix. The excellent outcomes demonstrated the potential of these membranes for more industrial gas separation applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S0016236123014539

35. Nawaz, M. A. H., Fazal, M. W., Akhtar, N., Nawaz, M. H., Hayat, A., & Yu, C. (2022). Multifunctional smart ZnSe-nanostructure-based fluorescent aptasensor for the detection of ochratoxin A. *Biosensors*, *12*(10), 844.

ABSTRACT:

Herein, we present a comprehensive investigation of rationally designed zinc selenide (ZnSe) nanostructures to achieve highly negatively charged ZnSe nanostructures. A Microwave-assisted hydrothermal synthesis method was used to synthesize three types of ZnSe nanostructures, i.e., nanorods, μ-spheres and nanoclusters, as characterized by a zeta potential analyzer, X-ray

diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy and BET, which were labeled as type A, B and C. Three different solvents were used for the synthesis of type A, B and C ZnSe nanostructures, keeping other synthesis conditions such as temperature, pressure and precursors ratio constant. Based on two heating time intervals, 6 and 9 h, types A, B and C were further divided into types A6, A9, B6, B9, C6 and C9. ZnSe nanostructures were further evaluated based on their fluorescent quenching efficiency. The maximum fluorescence quenching effect was exhibited by the ZnSe-B6 type, which can be attributed to its highly negative surface charge that favored its strong interaction with cationic dye Rhodamine B (Rh-B). Further, the optimized ZnSe-B6 was used to fabricate an aptasensor for the detection of a food-based toxin, ochratoxin-A (OTA). The developed aptasensor exhibited a limit of detection of 0.07 ng/L with a wide linear range of 0.1 to 200 ng/L.

Web URL: https://www.mdpi.com/2079-6374/12/10/844

36. Khan, S. I., Hassan, A., Bano, R., Gilani, M. A., Marty, J. L., Zhang, H., & Hayat, A. (2024). An innovative and universal dual-signal ratiometric spectro-electrochemical imprinted sensor design for sandwich type detection of anticancer-drug, gemcitabine, in serum samples; cross validation via computational modeling. Talanta, 267, 125233.

ABSTRACT:

An innovative and universal imprinted sensor design for sandwich type detection of gemcitabine (GMT) in human serum samples is described. GMT is widely used in the treatment of different tumors, such as lung, ovarian, pancreatic, and breast cancer. The serum albumin-drug interaction was translated to design a multifunctional, ratiometric and dual mode silver nanoparticle based probe (BSA-Ag nanoprobe), as a read out system. Subsequently, polypyrrol imprinted drug receptor sites was engineered to selectively capture the GMT on the transducer surface. The GMT was sandwiched between imprinted receptor surface and BSA-Ag nanoprobe to generate the spectro-electrochemical signals. The formation of nanoprobe was confirmed through various characterization techniques, including X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, micro-Raman spectroscopy, Dynamic light scattering (DLS), and UV–Visible (UV–Vis) analysis, while each step of sensor fabrication was characterized via field emission scanning electron microscope (FE-SEM), Static water Contact angle measurements, cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS). Different variable parameters were optimized to improve the analytical performance of the sensor design. Under optimal conditions, spectro-electrochemical sensor permitted linear ranges between 1 and 200 μmol L^{-1} and 0.5–200 μmol L^{-1}, with limits of detection (LOD) of 0.4 μmol L^{-1} and 0.15 μmol L^{-1} respectively. Furthermore, the designed sensor successfully differentiated the serum samples of lung cancer patients and healthy volunteers. The obtained results were validated with standard Liquid chromatography-mass spectrometry (LC/MS) analysis of the patients and healthy volunteer's serum samples. Lastly, density functional theory (DFT) and molecular docking calculations revealed the enhanced GMT binding capability of molecularly imprinted polypyrrole and molecular level interaction between the GMT and BSA, to validate the sandwich sensor design.

Web URL: https://www.sciencedirect.com/science/article/pii/S0039914023009840

37. Siddiqui, A. S., Ahmad, M. A., Nawaz, M. H., Hayat, A., & Nasir, M. (2022). Decorating Zirconium on Graphene Oxide to Design a Multifunctional Nanozyme for Eco-Friendly Detection of Hydrogen Peroxide. Catalysts, 12(10), 1105.

ABSTRACT:

Peroxidase enzymes are crucial in analytical chemistry owing to significant peroxide analytes and their key role in hydrogen peroxide (H_2O_2) detection. Therefore, exploiting appropriate catalysts for the peroxidase like reactions has become crucial for achieving desired analytical performance. Zirconium (Zr) has attracted growing interest, as a safe and stable potential eco-friendly catalyst for various organic transformations that address increasing environmental challenges. Hence, aiming at fast, sensitive and selective optical detection of H_2O_2, a colorimetric platform is presented here, based on the excellent peroxidase enzyme-like activity of Zr decorated on graphene oxide (GO). The synergistic effect achieved due to intimate contact between an enzyme like Zr and the high surface area 0f GO ensures efficient electron transfer that increases the chemical and catalytic activity of the composite and advances the decomposition of H_2O_2 into hydroxyl radicals. The designed probe, thus, efficiently catalyzes the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB), via hydroxyl radicals, thereby transforming the colorless TMB into blue oxidized TMB within 2 min. The catalytic mechanism of the Zr-GO enzyme mimic is proposed herein and verified using a fluorescent probe terephthalic acid (TA) and other scavenger experiments. The multifunctional optical probe allows sensitive and highly selective recognition of H_2O_2 in a linear range from 100 to 1000 µM with a low detection limit of 0.57 µM. Essentially, the direct accessibility of Zr prevents having to use the complicated preparation and purification procedures mostly practiced for conventional biozymes and nanozymes. The devised method offers several gains, including being green and an inexpensive catalyst, having lower LOD, being fast, cost-effective and sensitive, and having selective work-up procedures.

Web URL: https://www.mdpi.com/2073-4344/12/10/1105

38. Siddiqui, A. S., Ahmad, M. A., Nawaz, M. H., Hayat, A., & Nasir, M. (2022). Decorating Zirconium on Graphene Oxide to Design a Multifunctional Nanozyme for Eco-Friendly Detection of Hydrogen Peroxide. Catalysts, 12(10), 1105.

ABSTRACT:

Peroxidase enzymes are crucial in analytical chemistry owing to significant peroxide analytes and their key role in hydrogen peroxide (H_2O_2) detection. Therefore, exploiting appropriate catalysts for the peroxidase like reactions has become crucial for achieving desired analytical performance. Zirconium (Zr) has attracted growing interest, as a safe and stable potential eco-friendly catalyst for various organic transformations that address increasing environmental challenges. Hence, aiming at fast, sensitive and selective optical detection of H_2O_2, a colorimetric platform is presented here, based on the excellent peroxidase enzyme-like activity of Zr decorated on graphene oxide (GO). The synergistic effect achieved due to intimate contact between an enzyme like Zr and the high surface area 0f GO ensures efficient electron transfer that increases the chemical and catalytic activity of the composite and advances the decomposition of H_2O_2 into hydroxyl radicals. The designed probe, thus, efficiently catalyzes the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB), via hydroxyl radicals, thereby transforming

the colorless TMB into blue oxidized TMB within 2 min. The catalytic mechanism of the Zr-GO enzyme mimic is proposed herein and verified using a fluorescent probe terephthalic acid (TA) and other scavenger experiments. The multifunctional optical probe allows sensitive and highly selective recognition of H_2O_2 in a linear range from 100 to 1000 μM with a low detection limit of 0.57 μM. Essentially, the direct accessibility of Zr prevents having to use the complicated preparation and purification procedures mostly practiced for conventional biozymes and nanozymes. The devised method offers several gains, including being green and an inexpensive catalyst, having lower LOD, being fast, cost-effective and sensitive, and having selective work-up procedures.

Web URL: https://www.mdpi.com/2073-4344/12/10/1105

39. Siddiqui, A. S., Hayat, A., Pohan, L. G., Ahmad, M. A., & Nasir, M. (2023). Design of DMAP functionalized MoS2-GO hybrid for targeted visual detection of dopamine: a step towards chromogenic substrate free point of care testing. Materials Today Chemistry, 32, 101625.

ABSTRACT:

Abnormal release of DA, a crucial neurotransmitter, can cause serious neurological disorders such as Parkinson's and Alzheimer's disease. Thus, sensitive DA detection becomes critical for the investigation of physiological functions and disease diagnosis. Specific DA quantification in real samples is a tedious task due to the presence of analogous neurotransmitters. Therefore, aiming at on-site selective monitoring of DA, a high-performance colorimetric probe has been designed using a DMAP-modified MoS_2-GO hybrid for highly selective visual detection of DA, especially for POC testing. The efficient DA recognition can be attributed to the large surface area with potentially active sites for greater electron transport and oxidation ability owing to the synergistic effect of MoS_2 and GO. The hybrid has been modified with DMAP, which allows extremely selective and specific DA recognition against potential interferents, especially other neurotransmitters. The proposed mechanism relies on the attachment of DA to the hybrid surface, facilitating the oxidation and complexation processes that induce aggregation causing instant color change. The designed colorimetric method can recognize DA in neutral medium at room temperature without any reagents or supplementary operations. A good linear relationship was observed between the absorbance of the hybrid and DA concentrations in the range 1–100 μM, with a low detection limit of 0.17 μM. Furthermore, the applicability of the present approach was also verified by the analysis of DA in human serum samples and proved to be promising for sequential DA detection in biological samples with good precision and accuracy. From a POC perspective, easy-to-use paper-based test strips were prepared for visual recognition of DA in just 3 min. Results indicate that the designed DA assay provides a powerful, low-cost, convenient, and reagentless colorimetric platform for instant and highly selective DA detection in aqueous solution, strips, and human serum that is predicted to find extended applications in the fields of biosensing, clinical diagnosis, and in-vitro disease monitoring.

Web URL: https://www.sciencedirect.com/science/article/pii/S2468519423002525

40. Farooq, M., Hayat, A., Nawaz, M. H., Hassan, M. S., Nasir, M., & Ajab, H. (2023). Tuning the structure and properties of MoS2-SrTiO3 nanocomposite and its enzyme mimic

behavior for enhanced optical sensing and measurement of H2O2 in biological samples. Measurement, 216, 112901.

ABSTRACT:

In the present study a quick sensing assay was introduced based on novel biomimetic oxidase like behavior of Molybdenum Sulfide and Strontium Titanate (MoS_2-$SrTiO_3$) nanocomposite for colorimetric detection of H_2O_2. In order to improve the adhesion nanocomposite was encapsulated into the gel and loaded on the surface of filter paper. The synergistic effect of MoS_2 and $SrTiO_3$ on sensing exhibited the intrinsic peroxidase-like activity by catalyzing the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB) as substrate and as a result an improved naked eye response was observed. This enhanced response was well supported by characterizations techniques like FT-IR, SEM, XRD and Raman spectroscopy. For better sensitivity and selectivity, the following conditions like gel concentration (0.3 g/6mL) at room temperature, incubation time (30 min) and concentration of nanocomposite (2 mg/mL) were optimized. A better sensitivity was obtained with a lower limit of detection (LOD) of 0.08 μM in a relatively wide range of 0.1 μM to 5 μM and high correlation coefficient (R^2) of 0.978. The ability of the sensor in real samples like milk and tap water was assessed with good recovery values ranging from 91 − 98 % in the presence of interfering compounds. This colorimetric detection using filter paper modified with enzyme mimetic nanocomposites is a step forward towards the point of care devices for onsite detection and monitoring of the dieases which was otherwise quite difficult and expensive.

Web URL: https://www.sciencedirect.com/science/article/pii/S0263224123004657

41. Abid, S., Zulfiqar, S., Anjum, M. A., Bullock, A. J., MacNeil, S., & Yar, M. (2023). An alginate-Based tube gel delivering 2-deoxy-D-ribose for stimulation of wound healing. Journal of Biomaterials Applications, 38(2), 264-279.

ABSTRACT:

Developing multifunctional wound dressings capable of inducing rapid angiogenesis and with antibacterial activity would be attractive for diabetic and superficial wound healing. Hydrogels delivered from tubes have several desirable features -they are easy to apply, keep the wound moist, reduce the entry of microorganisms and avoid the need for painful dressing removal. Previously we reported that 2 deoxy-D-ribose (2dDR) delivered from a variety of dressings is capable of promoting wound healing by stimulating angiogenesis. Alginate hydrogels are an ideal vehicle to deliver a bioactive agent capable of promoting wound healing. In this study we developed and evaluated a tube hydrogel capable of delivering 2dDR with the aim of achieving a stable, convenient to administer and biologically effective wound treatment. Further, we included the stabilizer 2-phenoxy ethanol which provided antimicrobial activity. We synthesized hydrogels by the Green method, using simple mixing of sodium alginate, propylene glycol, 2-phenoxy ethanol and 2dDR in water. FTIR (Fourier transformation infrared spectroscopy) analysis confirmed an absence of undesirable chemical changes in the gel components, and SEM images of the freeze-dried gels showed porous structures. When 2dDR alginate gel (2dDR-SA hydrogel) was placed in PBS at 37°C, almost 92% of 2dDR was released within 7 days. When tested on cultured cells, 2dDR-SA hydrogels did not inhibit metabolic activity or proliferation,

achieving up to 90 and 98% of control respectively over 7 days. 2dDR-SA hydrogel also showed anti-bacterial activity against *E. coli, Pseudomonas aeruginosa, Staphylococcus aureus,* and *MRSA* which was attributable to the stabilizer 2-phenoxy ethanol in the hydrogel. Stimulation of angiogenesis in the chorioallantoic membrane assay by 2dDR-SA hydrogel was found to be significant compared to the blank-SA. Wound healing potential was studied in full-thickness wounds in rats where acceleration of wound healing was seen. H&E staining of the wound tissue showed an enhanced number of blood vessels and re-epithelization, and a reduced number of inflammatory cells in 2dDR-SA treated animals compared to blank-hydrogels while Masson's trichrome staining showed increased collagen deposition. In summary we describe a convenient to apply hydrogel which has promise for use in a range of superficial skin wounds including applications in chronic wound care.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/08853282231191218

42. Nisar, A., Tabassum, S., Ayub, K., Mahmood, T., AlMohamadi, H., Khan, A. L., ... & Gilani, M. A. (2023). Photoswitchable nonlinear optical properties of azobenzene-based supramolecular complexes: insights from density functional theory. Physical Chemistry Chemical Physics, 25(30), 20430-20450.

ABSTRACT:

Density functional theory (DFT) calculations were performed for a series of supramolecular assemblies containing azobenzene (Azo-X where X = I, Br and H) and alkoxystilbazole subunits to evaluate their electronic, linear and nonlinear optical properties. These assemblies are derivatives of azobenzene, obtained by the substitution of electron-withdrawing and electron-donating groups onto the molecular skeleton. The interaction energies (Eint) of all the designed supramolecular complexes (IA–IF, IIA–IIF and IIIA–IIIF) range from −1.0 kcal mol−1 to −7.7 kcal mol−1. The electronic properties of these hydrogen/halogen bond driven supramolecular assemblies such as vertical ionization energies (VIE), HOMO–LUMO energy gap (GH–L), excitation energies, density of states (DOS) and natural population (NPA) analyses were also computed. The non-covalent interaction index (NCI) and quantum theory of atoms in molecules (QTAIM) analyses were also performed to validate the nature of inter- and intra-molecular interactions in these complexes. A substantial enhancement in the first hyperpolarizability (β0) values of the designed supramolecular complexes was observed, which is driven by the charge transfer from the pyridyl moiety of alkoxystilbazole to Azo-X. The highest β0 value of 1.3 × 104 au was observed for the supramolecular complex of p-nitro substituted azobenzene with alkoxystilbazole (ID complex). Moreover, the results show that the substitution of electron-withdrawing groups on Azo-X can also bring larger β0 values for such complexes. It was confirmed on a purely theoretical basis that both the types of noncovalent interactions present and the substituent group incorporated influence the nonlinear optical (NLO) response of the systems. Furthermore, the β0 values of the E (trans) and Z (cis) forms were compared to demonstrate the two-way photoinduced switching mechanism.

Web URL: https://pubs.rsc.org/en/content/articlelanding/2023/cp/d3cp01498c/unauth

43. Lone, S. B., Zeeshan, R., Khadim, H., Khan, M. A., Khan, A. S., & Asif, A. (2024). Synthesis, monomer conversion, and mechanical properties of polylysine based dental composites. Journal of the Mechanical Behavior of Biomedical Materials, 151, 106398.

ABSTRACT:

Objective

The aim of this study was to synthesize a new bioactive and antibacterial composite by incorporating reactive calcium phosphate and antibacterial polylysine into a resin matrix and evaluate the effect of these fillers on structural analysis, degree of monomer conversion, mechanical properties, and bioactivity of these newly developed polypropylene based dental composites.

Methodology

Stock monomers were prepared by mixing urethane dimethacrylate and polypropylene glycol dimethacrylate and combined with 40 wt% silica to make experimental control (E-C). The other three experimental groups contained a fixed percentage of silica (40 wt%), monocalcium phosphate monohydrate, and β-tri calcium phosphate (5 wt% each) with varying amounts of polylysine (PL). These groups include E-CCP0 (0 wt% PL), E-CCP5 (5 wt% PL) and E-CCP10 (10 wt% PL). The commercial control used was Filtek™ Z250 3M ESPE. The degree of conversion was assessed by using Fourier transform infrared spectroscopy (FTIR). Compressive strength and Vicker's micro hardness testing were evaluated after 24 h of curing the samples. For bioactivity, prepared samples were placed in simulated body fluid for 0, 1, 7, and 28 days and were analyzed using a scanning electron microscope (SEM). SPSS 23 was used to analyze the data and one-way ANOVA and post hoc tukey's test were done, where the significant level was set ≤0.05.

Web URL: https://www.sciencedirect.com/science/article/pii/S175161612400030

44. Jalal, A., Ahmad, S., Shah, A. T., Hussain, T., Nawaz, H. A., & Imran, S. (2024). Preparation of celecoxib loaded bioactive glass chitosan composite hydrogels: a simple approach for therapeutic delivery of NSAIDs. Biomedical Materials, 19(3), 035031.

ABSTRACT:

Arthritis causes inflammatory damage to joints and connective tissues. In the treatment of arthritis, precise and controlled drug delivery to the target site is among the frontline research approaches. In the present research work, celecoxib drug and bioactive glass incorporated chitosan hydrogels were fabricated by the freeze gelation method. Fourier transform infrared spectroscopy, scanning electron microscopy, and thermogravimetric analysis/differential scanning calorimetry techniques were used to characterize the hydrogels. Different kinetic models were applied to study the drug release kinetics. The celecoxib release was mainly controlled by a Fickian diffusion process followed by the Higuchi model. Maximum 86.2% drug entrapment was observed in 20 mg drug-loaded hydrogel and its swelling ratio was 115.5% in 28 d. Good hydrophilicity, good drug entrapment efficiency, and moderate drug release patterns of hydrogels can make them suitable for sustained drug release. The cytocompatibility of hydrogels was established by performing an MTT assay on the BHK-21 fibroblast cell line. The promising

results have proved that hydrogels can be considered potential material for the slow release of anti-inflammatory drug at the target site in arthritis.

Web URL: https://iopscience.iop.org/article/10.1088/1748-605X/ad3706/meta

45. Sajjad, S., Görke, O., Kocak, F. Z., Shumail, M., Tehseen, S., Zahid, S., ... & Tufail Shah, A. (2024). Acetanilide-loaded injectable hydrogels with enhanced bioactivity and biocompatibility for potential treatment of periodontitis. Journal of Applied Polymer Science, 141(14), e55200.

ABSTRACT:

Chronic periodontitis poses long-term challenges in dentistry, requiring the development of innovative dental composites with biocompatibility, bone regeneration, and antibacterial properties. This study focuses on synthesis of novel injectable thermoresponsive hydrogels composed of chitosan, sodium bicarbonate, bioactive glass (20 and 40% w/w), and acetanilide drug (0.3 and 0.6% w/w). These hydrogels exhibit a sol–gel transition at 37°C, addressing periodontal challenges with reduced gelation time. The smooth flow characteristic was evaluated through 17-22 gauge syringe needles at low temperature. Rheological studies demonstrated pseudoplastic behavior, with viscosity decreasing as shear rate increases. Fourier transform infrared and x-ray diffraction analysis confirmed the bioactivity of hydrogels, forming a bone-like apatite layer in simulated body fluid. The drug-loaded hydrogels demonstrated promising in vitro antibacterial properties against dental pathogens, specifically *Staphylococcus aureus* and *Pseudomonas aeruginosa*. Drug dissolution analysis revealed relatively high release rate at 37°C, highlighting its role in rapidly eliminating bacterial colonies at the target site, while the subsequent sustained release contributes to the prevention of infection recurrence. Finally, biocompatibility was assessed with fibroblast, where the cells were observed anchoring into the polymeric chains of hydrogel through extended filopodia.

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/app.55200

46. Liang, J., Li, C., Mo, J., Iwata, H., Rehman, F., Song, J., & Guo, J. (2024). Metatranscriptomic profiles reveal the biotransformation potential of azithromycin in river periphyton. Water Research, 251, 121140.

ABSTRACT:

Assessment of the interaction between the biotransformation of chemical contaminants and enzyme activity from aquatic microbial communities is critical for improving the micropollutant degradation in river remediation. Here, association mining based on metatranscriptomic analysis was initially applied to determine the genes encoding enzymes involved in the azithromycin (AZI) transformation process and the corresponding microbial hosts in periphyton, followed by revealing the dynamic variation in the community structure and function. In terms of the biotransformation potential, the highly correlated 15 enzymes were suggested to be primarily involved in AZI biotransformation, energy supply, and antibiotic resistance processes, especially aryl-alcohol dehydrogenases (EC: 1.1.1.90), hydroxylamine dehydrogenase (EC: 1.7.2.6), and monooxygenases (EC: 1.14.11.57) that were involved in the biotransformation of AZI. In the matter of community ecological function, the photosystem II (PSII) reaction center in the periphytic photosynthetic process,

as indicated by Fv/Fm, was inhibited after AZI exposure, which may be attributed to the down-regulated genes enriched in the photosynthesis - antenna proteins (ko00196), photosynthesis (ko00195), and two-component system (ko02020) pathways. Furthermore, the periphytic utilization capacity for carbohydrates and phenolic acids was enhanced, which was in accordance with all the increased expression of transcripts involved in the corresponding molecular pathways, including aminobenzoate degradation (ko00627), starch and sucrose metabolism (ko00500), ABC transporters (ko02010), phosphotransferase system (ko02060), galactose metabolism (ko00052), amino sugar and nucleotide sugar metabolism (ko00520). Taken together, this study highlighted the critical role of river periphyton in the micropollutant degradation and unraveled the molecular mechanism of antibiotic biotransformation as well as the structural and functional damage in the periphyton.

Web URL: https://www.sciencedirect.com/science/article/pii/S004313542400040X

47. Draz, M. U., Haq, M. Z. U., Hayat, A., & Ajab, H. (2024). An ALP enzyme-based electrochemical biosensor coated with signal-amplifying BaTiO 3 nanoparticles for the detection of an antiviral drug in human blood serum. Nanoscale Advances, 6(2), 534-547.

ABSTRACT:

Tenofovir (TFV) is an antiviral drug used to treat the co-infections of HIV/HBV viruses. Accurate monitoring of TFV drug levels is essential for evaluating patient adherence, optimizing dosage, and assessing treatment efficacy. Herein, we propose an innovative electrochemical sensing approach by using the alkaline phosphatase (ALP) enzyme with the support of BaTiO3 nanoparticles. An attractive sensitivity and selectivity of the developed sensor towards TFV detection were achieved. First, the nanoparticles were synthesized by following a single-step sol–gel method and characterized through various analytical techniques, including SEM, EDX, FT-IR, BET, zeta potential, XRD, and UV-vis and Raman spectroscopy. The suggested mechanism demonstrated the formation of a strong bond between TFV and the ALP enzyme, primarily through the phosphate group, resulting in enzyme inhibition. Various parameters like nanoparticle amount, electrode modification time with enzyme and BaTiO3 nanoparticles, and drug incubation time were optimized. The biosensor demonstrated an outstanding limit of detection (LOD) of 0.09 nM and recovery percentages of 98.6–106% in human blood serum, indicating adequate repeatability and selectivity. The proposed biosensor can be converted into a portable device for measuring small sample volumes and observing patients for immediate medical care or personalized therapies. It achieved better sensitivity compared to existing methods, making it suitable for precise drug detection in microdoses.

Web URL: https://pubs.rsc.org/en/content/articlehtml/2024/na/d3na00839h

48. Jubeen, F., Batool, A., Naz, I., Sehar, S., Sadia, H., Hayat, A., & Kazi, M. (2024). Mycotoxins detection in food using advanced, sensitive and robust electrochemical platform of sensors: A review. Sensors and Actuators A: Physical, 115045.

ABSTRACT:

Mycotoxins constitute a grave threat to human health and life by causing significant losses in healthcare and trade and by contaminating food and feed. Diverse matrices and trace concentrations of mycotoxins in food make measurement and identification challenges, necessitating highly sensitive and specialized detection methods. Most nations, particularly the European Union, have implemented preventative programs to reduce contamination and stringent legislation about the permitted amounts in foods. Official methods of mycotoxin analysis typically require sophisticated instrumentation. Electrochemical (EC) sensors have emerged as a viable method for addressing specificity and sensitivity in detection due to their ease of use, exceptional sensitivity, low cost, and ease of miniaturization. Here is an overview of recent studies using electrochemical sensors and biosensors for mycotoxin detection for food safety. First, we summarize the conventional methods used for the monitoring of mycotoxins in food. Then, state-of-the-art electrochemical sensors for detecting noxious mycotoxins are discussed. The classification of various electrochemical detection techniques led to detailed descriptions of design strategies, recognition mechanisms, and probe materials. This review provides critical inspiration for future applications of electrochemical analysis and point-of-care testing for mycotoxins.

Web URL: https://www.sciencedirect.com/science/article/pii/S0924424724000384

49. Asghar, H., Bilal, S., Nawaz, M. H., Rasool, G., & Hayat, A. (2024). Host–Guest Mechanism via Induced Fit Fullerene Complexation in Porphin Receptor to Probe Salivary Alpha-Amylase in Dental Caries for Clinical Applications. ACS Applied Bio Materials, 7(2), 1250-1259.

ABSTRACT:

Salivary α-amylase is the most abundant protein of human saliva that potentially binds to streptococcus and other bacteria via specific surface-exposed α-amylase-binding proteins and plays a significant role in caries development. The detection of α-amylase in saliva can be used as a bioindicator of caries development. Herein, a facile strategy has been applied, tailoring the photochemical properties of 5,10,15,20-tetrakis(4-hydroxyphenyl)-21*H*,23*H*-porphine (TPPOH) and the fullerene C60 complex. The fluorescence emission of TPPOH is quenched by starch-coated fullerene C60 via charge-transfer effects, as determined by UV absorption and fluorescence spectroscopic studies. The starch-coated C60 has been thoroughly characterized via Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), optical microscopy, thermal gravimetric analysis (TGA), static water contact angle measurements, and zeta potential measurements. The analytical response of the assay showed a linear fluorescent response in α-amylase concentrations ranging from 0.001–0.1 Units/mL, with an LOD of 0.001 Units/mL. The applicability of the method was tested using artificial saliva with quantitative recoveries in the range 95–100%. The practicability of the procedure was verified by inspecting saliva samples of real clinical samples covering all age groups. We believe that the proposed method can serve as an alternative analytical method for caries detection and risk assessment that would also minimize the cost of professional preventive measures and treatments.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsabm.3c01189

50. Tariq, A., Arif, A., Akram, M., Latif, U., Nawaz, M. H., Andreescu, S., ... & Hayat, A. (2024). Tailoring molecular recognition in predesigned multifunctional enzyme mimicking porphyrin imprinted interface for high affinity and differential selectivity; sensing etoposide in lung cancer patients. Biosensors and Bioelectronics, 245, 115833.

ABSTRACT:

Nanozymes are cost-effective and robust but they lack specificity and selectivity, limiting their potential practical applications. Herein, molecularly imprinted polymers (MIPs) were grown in combination with multifunctional 5,10,15,20-tetrakis(4-hydroxyphenyl)-21H,23H-porphyrin (THPP) oxidase-like nanozyme to engineer THPP@MIP interface with high affinities and differential selectivity for structurally related target analytes. THPP nanozyme displayed a high level of predefined binding affinity for etoposide (ETO), and served as a predesigned functional monomer to rationally tailor the selectivity of THPP@MIP surface in the presence of different guest molecules. THPP nanozyme in combination with conventional monomers was imprinted on a portable and disposable cellulose paper matrix under UV light to create a UV-cured imprinted interface for optical detection of ETO. The THPP@MIP enzyme mimicking interface, having ETO specific and selective target recognition pockets, catalyzed the oxidation of colorless 3,3′,5,5′-tetramethylbenzidine (TMB) to generate visible blue oxidized TMB (oxTMB) without exogenous hydrogen peroxide (H_2O_2). The ETO binding on the THPP@MIP surface blocked the channels for TMB access to THPP cavities. The THPP@MIP sensor permitted to detect ETO in the linear range of 0.005–10 μg mL^{-1}, with a limit of detection (LoD) of 0.002 μg mL^{-1}, and showed a remarkable specificity and selectivity against other drug molecules. Furthermore, the THPP@MIP sensor successfully differentiated the serum samples of lung cancer patients and healthy volunteers. The obtained results were validated with standard High performance liquid chromatography-mass spectrometry (HPLC/MS) analysis of the serum samples. Additionally, ETO injection/infusion solutions and ETO-free serum samples were used to perform the matrix effect and recovery studies. This work demonstrates that molecular imprinting with predesigned, enzyme mimicking, high-affinity functional monomer can serve as a highly selective and specific universal interface for broad spectrum sensing applications in various analytical domains.

Web URL: https://www.sciencedirect.com/science/article/pii/S0956566323007753

51. Nawaz, M. A. H., Nazari, E., Akhtar, M. H., Rad, V. F., Zhang, H., Moradi, A. R., & Hayat, A. (2024). Probing aptamer-mucin 1 binding events on polydopamine@ carbon nanotubes modified cellulose paper interface using speckle pattern analysis for label free aptasensing. Microchemical Journal, 199, 109994.

ABSTRACT:

Herein, we have developed a cellulose paper-based aptasensing protocol by employing dynamic laser speckle (DLS) analysis for direct and label-free probing of the binding interface. Cellulose filter paper surface was modified by using the mussel adhesion chemistry of polydopamine modified carbon nanotubes (PDA@CNTS). The mussel chemistry resulted in strong adhesion and binding of PDA@CNTs on cellulose paper surface. The modified surface was subsequently

employed in the construction of label free aptasensor for detection of cancer biomarker mucin 1 (MUC1). Taking advantage of DLS technique, it provided us with sensitive and accurate analysis of target biomarker MUC1 by the intrinsic randomness of patterns generated from cellulose based paper surface. The developed aptasensor was evaluated using DLS at various fabrication steps, where the scattered laser beams from these samples were collected and analyzed based on the obtained speckle patterns. Under the optimal experimental conditions, paper-based aptasensor achieved sensitive and selective detection of MUC1, exhibiting excellent linear range (15–100) μM with a limit of detection of 1 μM. This work presents a novel study of promising laser speckle paper-based aptasensor, providing new insights for the development of low-cost, sensitive, and portable paper-based analytical tools for biological applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S0026265X24001061

52. Wang, T., Cai, S., Wu, J., Jiang, C., Xiao, Z., Akram, M., ... & Tian, Y. (2024). A flexible nanofiber membrane containing dendritic oxygen probe for visual monitoring pressure distribution. Talanta, 274, 125977.

ABSTRACT:

Pressure-sensitive paints (PSP) enable non-intrusive visualization of surface pressure distribution on model surface which is important for aerodynamic studies. However, conventional PSP materials suffer from photobleaching and inadequate sensitivity. In this work, we rationally designed and synthesized novel dendritic oxygen probes (**PT1** and **PT2**) by covalently grafting fluorinated dendrons onto platinum tetrakis(pentafluorophenyl)porphyrin (**PT0**) (a common oxygen probe). Subsequently, **PT2** loaded nanofibers membranes from polycaprolactone (PCL) were fabricated by electrospinning. Fabricated membranes showed high oxygen sensitivity (I_0/I_{100} = 35.3) with excellent flexibility, good reversibility, and outstanding photostability (merely 2.0% intensity loss after prolonged irradiation). The pressure sensitivity was found around 0.73 % per kilopascal. Furthermore, significant variation in emission intensity with respect to the variation in air pressure (1.3–101.32 kPa), facilitates the naked eye visualization of the pressure distribution on the membrane surface. Such excellent oxygen and pressure sensitivity and photostability might be due to high fluorine contents of complex dendritic structure of **PT2**. This flexible fluorine-functionalized dendritic oxygen probe puts forward a facile and effective strategy to develop advanced PSP materials enabling accurate pressure mapping for aerodynamic studies.

Web URL: https://www.sciencedirect.com/science/article/pii/S0039914024003564

53. Tariq, S., Shah, S. A., Hameed, F., Mutahir, Z., Khalid, H., Tufail, A., ... & Khan, A. F. (2024). Tissue engineered periosteum: Fabrication of a gelatin basedtrilayer composite scaffold with biomimetic properties for enhanced bone healing. International Journal of Biological Macromolecules, 263, 130371.

ABSTRACT:

The periosteum, a vascularized tissue membrane, is essential in bone regeneration following fractures and bone loss due to some other reasons, yet there exist several research gaps concerning its regeneration. These gaps encompass reduced cellular proliferation and bioactivity, potential toxicity, heightened stiffness of scaffold materials, unfavorable porosity, expensive materials and procedures, and suboptimal survivability or inappropriate degradation rates of the implanted materials. This research used an interdisciplinary approach by forming a new material fabricated through electrospinning for the proposed application as a layer-by-layer tissue-engineered periosteum (TEP). TEP comprises poly(ε-caprolactone) (PCL), PCL/gelatin/magnesium-doped zinc oxide (vascular layer), and gelatin/bioactive glass/COD liver oil (osteoconductive layer). These materials were selected for their diverse properties, when integrated into the scaffold formation, successfully mimic the characteristics of native periosteum. Scanning electron microscopy (SEM) was employed to confirm the trilayer structure of the scaffold and determine the average fiber diameter. In-vitro degradation and swelling studies demonstrated a uniform degradation rate that matches the typical recovery time of periosteum. The scaffold exhibited excellent mechanical properties comparable to natural periosteum. Furthermore, the sustained release kinetics of COD liver oil were observed in the trilayer scaffold. Cell culture results indicated that the three-dimensional topography of the scaffold promoted cell growth, proliferation, and attachment, confirming its non-toxicity, biocompatibility, and bioactivity. This study suggests that the fabricated scaffold holds promise as a potential artificial periosteum for treating periostitis and bone fractures.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813024011747

54. Younas, M., Yar, M., AlMohamadi, H., Mahmood, T., Ayub, K., Khan, A. L., ... & Gilani, M. A. (2024). A rational design of covalent organic framework supported single atom catalysts for hydrogen evolution reaction: a DFT study. International Journal of Hydrogen Energy, 51, 758-773.

ABSTRACT:

Excessive consumption of fossil fuels and CO_2 emissions exacerbate global environmental concerns. Unfortunately, fossil fuel reserves are dwindling and fossil fuel energy is unsustainable, non-renewable, and costly. Due to these concerns, there is an imperative demand for eco-friendly energy conversion electrochemical systems. Hydrogen (H_2) is ubiquitously regarded as a fossil fuel substitute and a potential sustainable energy source. Water electrolysis powered by renewable resources is being considered as a sustainable approach to produce H_2. To cater the need, electrocatalysts with non-precious single metal atoms supported on a covalent organic framework (TM@COF SACs) have been proposed for HER. Single atoms of Co, Ni, Cu, and Zn were introduced onto the COF substrate. The thermodynamic stability, HOMO, LUMO energies, HOMO-LUMO energy gaps, DOS spectra, and change in the Gibbs free energy of adsorbed atomic hydrogen (ΔG_{H*}) on the catalyst's surface are used to evaluate the catalytic performance of designed complexes for HER. Among all the considered complexes, Zn@COF demonstrated the highest potential to act as a single atom catalyst, with an E_{int} value of −0.11 eV. Density functional theory (DFT) findings suggest that single Zn atom doped on the surface of the covalent organic framework with ΔG_{H*} value of −0.88 eV has a substantial effect on the performance of the HER. This research opens up new possibilities for the advancement and

utilization of highly efficient, stable, and cost-effective single-atom catalysts for HER, thereby laying the foundation for future developments in this field.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360319923034559

55. Liu, X., Chen, F., Saeed, M., Li, X., Zhang, H., Zhang, J., ... & Yu, H. (2024). In-situ vaccination immunotherapy of colorectal cancer with STING agonist-integrated supramolecular nanovectors. Nano Today, 56, 102273.

ABSTRACT:

The immunosuppressive tumor immune microenvironment and low tumor immunogenicity invariably subvert the efficacy of cancer vaccine and the antitumor immunity. An alternative approach to improve cancer vaccination immunotherapy is to synergistically trigger stimulator of interferon genes (STING) activation for transforming immunologically 'cold' tumor into 'hot' tumor. Herein, we presented a supramolecular nanovector (namely HCCSM) integrating with the chemotherapeutic agent camptothecin (CPT) and STING agonist MSA-2 for in-situ vaccination immunotherapy of colorectal cancer. The nanovector was prepared via well-tunable host-guest complexation of cyclodextrin-grafted hyaluronic acid with MSA-2 and adamantine-conjugated prodrug of CPT. Upon intravenous injection, HCCSM achieved active tumor targeting by recognizing highly expressed CD44 on colorectal tumor cells, and specifically co-delivered CPT and MSA-2 into tumors. CPT effectively induced immunogenic cell death (ICD) of tumor cells and triggered tumor-associated antigens (TAAs) release at the tumor site. Subsequently, tumor infiltrating-dendritic cells captured TAAs and MSA-2 to enhance antigen cross-presentation through the activation of STING pathway and secretion of type-I interferon. HCCSM elicited robust antitumor immunity and thus exhibited remarkable therapeutic benefit in primary and distant CT26 colorectal tumors. Our developed nanovector represents an effective combination strategy for vaccination immunotherapy of colorectal cancer.

Web URL: https://www.sciencedirect.com/science/article/pii/S1748013224001282

56. Tabassum, S., Saqib, M., Batool, M., Sharif, F., Gilani, M. A., & Huck, O. (2024). Eco-friendly synthesis of mesoporous bioactive glass ceramics and functionalization for drug delivery and hard tissue engineering applications. Biomedical Materials, 19(3), 035014.

ABSTRACT:

Hard tissue regenerative mesoporous bioactive glass (MBG) has traditionally been synthesized using costly and toxic alkoxysilane agents and harsh conditions. In this study, MBG was synthesized using the cheaper reagent SiO 2 by using a co-precipitation approach. The surface properties of MBG ceramic were tailored by functionalizing with amino and carboxylic groups, aiming to develop an efficient drug delivery system for treating bone infections occurring during or after reconstruction surgeries. The amino groups were introduced through a salinization reaction, while the carboxylate groups were added via a chain elongation reaction. The MBG, MBG-NH2, and MBG-NH-COOH were analyzed by using various techniques: x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller (BET), scanning electron microscopy and energy-dispersive x-ray spectroscopy. The XRD results confirmed the successful preparation of MBG, and the FTIR results indicated successful

functionalization. BET analysis revealed that the prepared samples were mesoporous, and functionalization tuned their surface area and surface properties. Cefixime, an antibiotic, was loaded onto MBG, MBG-NH2, and MBG-NH-COOH to test their drug-carrying capacity. Comparatively, MBG-NH-COOH showed good drug loading and sustained release behavior. The release of the drug followed the Fickian diffusion mechanism. All prepared samples displayed favorable biocompatibility at higher concentration in the Alamar blue assay with MC3T3 cells and exhibited the good potential for hard tissue regeneration, as carbonated hydroxyapatite formed on their surfaces in simulated body fluid.

Web URL: https://iopscience.iop.org/article/10.1088/1748-605X/ad2c19/meta

DEPARTMENT OF MANAGEMENT SCIENCES

1. Rana, M. L. T., & Alvi, T. H. (2023). Retailers-Led Brand Value Co-Creation Behaviors: An Intervening Analysis. Journal of Development and Social Sciences, 4(2), 589-603.

ABSTRACT:
There has been ample research on brand value co-creation (BVCC), but majorly it involved only one stakeholder (i.e., customers) as the source of co-creation. This paper aims to study employees' brand citizenship behaviors (EBCB) with retailers' brand value co-creation behaviors with a mediation mechanism of brand attachment in the FMCG sector. Scales were adapted from previous studies to measure EBCB, brand attachment, retailer-led feedback, retailer-led advocacy, and retailer-led helping. Data were collected through self-administered questionnaires, and PLS-SEM was used to analyze a sample of 189 salespersons and retailers. The findings support the complimentary partial mediation role of brand attachment in fostering retailers' BVCC behaviors by EBCB. This study offers comprehensive insights into employees' behaviors in cultivating retailers' co-creation behaviors. Firms and marketers may benefit by focusing on the behaviors of their employees, especially sales employees who frequently visit retail stores.

Web URL: https://www.ojs.jdss.org.pk/journal/article/view/512

2. Sarfraz, M., Hussain, G., Nazir, M. S., Abdullah, M. I., & Rashid, M. A. (2023). The moderating role of industry clockspeed on the relation between supply chain integration practices and new product flexibility. Heliyon, 9(3).

ABSTRACT:
This study assessed the firm's new product flexibility in the recovery phase of COVID-19. Using the theoretical lens of organizational information processing theory, it established the

relationship between supply chain integration practices (supply chain planning, internal integration, and supplier involvement) and new product flexibility. It also explained the moderating effect of industry clockspeed on supply chain integration practices and new product flexibility with the help of contingency theory. This study used an online survey method to collect data from plant managers, and we received 256 useable responses. We conducted a confirmatory factor analysis to test the validity and reliability of the scales, and we tested hypotheses using moderated multiple regression technique. The results showed significant positive relationships between supply chain integration practices and new product flexibility. The moderating effects hypotheses showed that industry clockspeed significantly and positively moderated on supply chain planning-new product flexibility and internal integration-new product flexibility links. But it negatively moderated on supplier involvement and new product flexibility. Our study departs from earlier studies in the field that were conducted under normal circumstances. We conducted our study in the recovery phase of COVID-19 in Pakistan, when firms, after fourteen days of complete lockdown, resumed their operations and experienced a new business landscape.

Web URL: https://www.cell.com/heliyon/pdf/S2405-8440(23)01690-0.pdf

3. Javed, U., Rashid, M. A., Hussain, G., & Shafique, S. (2023). Consumers' perception of green brand attributes and its outcomes: a sustainable perspective. Journal of Environmental Planning and Management, 1-23.

ABSTRACT:

The resurgence of green marketing engrossed the phenomenon of greenwashing, misleading and deceiving consumers with false claims about the firms' environmental practices. Drawing on attribution theory, this study examines the direct relationship between perceived greenwashing (PGW) and brand credibility (BC) and indirect relationship through green skepticism (GSP). The study also examines the moderating effect of environmental concern (EC) based on contingency theory in both direct and indirect relationships. Data were collected through self-administered questionnaires from consumers and 508 usable responses were analyzed. The study's hypotheses were tested using PROCESS macro for SPSS. The results show that PGW is negatively related to BC both directly and indirectly via GSP, whereas EC moderated, directly and indirectly, the relationships between PGW and BC, suggesting that the relationship between PGW and BC is fostered when EC is high. This study helps managers to understand how overstated/deceptive green claims may lead to destructive consequences for the company.

Web URL: https://www.tandfonline.com/doi/full/10.1080/09640568.2023.2178882

4. Sultan, M., Hussain, G., Ismail, W. K. W., & Rashid, M. A. (2023). From entrepreneurial leadership to new product development performance: A study of the Coleman bathtub model. European Journal of Innovation Management.

ABSTRACT:

Purpose

This study aims to examine the relationship between entrepreneurial leadership (EL) and new product development performance (NPDP) at the firm level (level 2) of analysis and employee's creativity (EC) at the cross level (level 1) of analysis. It also examines the serial mediations of (1) intrinsic motivation (IM)-EC and (2) creative self-efficacy (CSE)-EC on the relationship between EL and NPDP.
Design/methodology/approach
A systematic random sampling technique was used to collect data through self-administered surveys from leaders and employees of small and medium-sized enterprises (SMEs) in Pakistan's IT sector. Analysis was conducted on net responses from 114 leaders and 476 employees.
Findings
The results revealed significant positive associations between EL and NPDP at the firm level of analysis and EC at the cross level of analysis. The results of the cross-level serial mediations show that (1) IM and EC, and (2) CSE and EC serially mediate the relationship between EL and NPDP.
Originality/value
This study is among the few to use the Coleman bathtub model to show top-down and bottom-up relationships. The study extends and complements the multilevel perspective on leadership and new product development research by simultaneously examining the relationships between EL and NPDP at the individual and firm levels.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/EJIM-12-2022-0723/full/html

5. Hussain, G., Nazir, M. S., Rashid, M. A., & Sattar, M. A. (2023). From supply chain resilience to supply chain disruption orientation: the moderating role of supply chain complexity. Journal of Enterprise Information Management, 36(1), 70-90.

ABSTRACT:
Purpose
This study aims to examine the direct and indirect effects of supply chain resilience enablers on supply chain disruption orientation per supply chain resilience. It conjointly examined the moderation of supply chain complexity on resilience enablers and supply chain resilience. It further detailed the conditional indirect effects of supply chain resilience enablers on supply chain disruption orientations via supply chain resilience at varying levels of supply chain complexity.
Design/methodology/approach
This study employed a time-lagged design (three-wave) and self-administered surveys to collect data from the supply chain managers of fast-moving consumer goods firms. A sample of 214 responses was used to test the hypothesized relationships.
Findings
The results showed that supply chain resilience significantly mediated on the relationship between supply chain resilience enablers and supply chain disruption orientation. Further, supply chain complexity positively moderated on supply chain resilience enablers and supply chain resilience. The results also supported the moderated mediated hypothesis.
Research limitations/implications

This study contributes to prevalent theory and practices in the wake of recent disruptions faced by the firms. It persuades the managers to emphasize on structuring resilient supply chain system to recover from the disruptions and accumulate and incorporate learning gained from the disruptions to strengthen the firm's response management system.

Originality/value

This study attempted to explore the underlying antecedents and consequences of supply chain resilience in Pakistan and established boundary condition effects of supply chain complexity on the proposed relationships. This research complemented and extended the conceits of resource-based and contingent resource-based views.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/jeim-12-2020-0558/full/html

6. Sarfraz, M., Abdullah, M. I., Mumtaz, N., Ibn-Ul-Hassan, S., & Ozturk, I. (2023). The effect of entrepreneurs' personality on entrepreneurial marketing in textile sector: the mediating role of self-efficacy. Industria Textila, 74(2), 230-237.

ABSTRACT:

The effect of entrepreneurs' personality on entrepreneurial marketing in textile sector: the mediating role of self-efficacy The study objective is to analyse the effect of big-five entrepreneurs' personality traits on entrepreneurial marketing while considering the mediating role of self-efficacy. Data were collected through a structured questionnaire; a study of 199 usable questionnaires out of 290 was carried out among young entrepreneurs. Structural equation modelling was used to test the study hypothesis. The results show a significant relationship between personality traits and entrepreneurial marketing. Openness, Extroversion, and Agreeableness personality traits are positively linked with entrepreneurial marketing. The findings also show a positive association between self-efficacy and entrepreneurial marketing. The current study contributes to the literature by analysing an entrepreneur's personality characteristics in entrepreneurial marketing.

Web URL:
http://revistaindustriatextila.ro/images/2023/2/13%20MUDDASSAR%20SARFRAZ%20INDUSTRIA%20TEXTILA%20no.2_2023.pdf

7. Mumtaz, B., Azhar, A., Abdullah, M. I., & Khan, A. A. (2023). Examining the relationship of paternalistic leadership, extent of centralisation and employee's voice behaviour. International Journal of Work Organisation and Emotion, 14(1), 101-118.

ABSTRACT:

Among many leadership approaches in Asia, literatures failed to gauge applicability of paternalistic leadership in Pakistani organisations. This research stresses on discussing how voice varies across the triad model of paternalistic leadership styles, power distance orientation, their interactions, and extent of centralisation. Data was collected from a sample of 324 employees, which includes 146 employees from public and 178 employees from private universities and

banks. The proposed hypotheses were tested by using confirmatory factor analysis followed by multiple regression analysis. The findings showed that employees' voice behaviour was negatively associated with authoritarian paternalism; positively associated with benevolent and moral paternalism; and negatively associated with extent of centralisation. Also, the positive relationship of benevolent paternalism and employees' voice behaviour was stronger when employees experience high levels of power distance, thereby accepting the proposed hypotheses. However, contrary to the propositions, no significant results were obtained regarding power distance moderating negative authoritarian and positive moral paternalist link with voice behaviour. Implications of findings and future research prospects are discussed.

Web URL: https://www.inderscienceonline.com/doi/abs/10.1504/IJWOE.2023.130243

8. Abdullah, M. I., Sarfraz, M., Ivascu, L., Ghafoor, S., & Ozturk, I. (2023). AN EMPIRICAL STUDY ON CONSUMER'S PURCHASE INTENTIONS TOWARD ONLINE SHOPPING IN PAKISTAN. ACTA TECHNICA NAPOCENSIS-Series: APPLIED MATHEMATICS, MECHANICS, and ENGINEERING, 65(3S).

ABSTRACT:

This research explores the effects of electronic word-of-mouth (e-WOM) information, attitude toward information (ATT), and purchasing. Subjective norms (SN), perceived behavioral control (PBC), and consumer's internet experience (CIE) on consumers' online purchasing intentions while considering the moderating role of information quality. A self-administered survey was conducted on customers in Pakistan. Based on the data collected from 330 consumers. This study carried the regression, descriptive analysis, Cronbach alpha, and correlation using SPSS and structural equation modeling (SEM) approach using AMOS. Study results reveal that e-WOM, ATT, SN, PBC, and CIE positively influence consumers' online purchasing intention. In particular, a new finding of the study highlights the importance of the moderating role of information quality. Moderating impacts were positive and significant in enhancing the relationships of e-WOM, ATT, SN, PBC, CIE, and PI. Firms and marketers must concentrate on online communication channels to affect consumers' intention toward purchasing online and engage in e-WOM communication. Companies should pay more attention to consumers' need for accurate and reliable information to enhance e-WOM and information influence.

Web URL: https://atna-mam.utcluj.ro/index.php/Acta/article/view/1932

9. Sarwar, A., Abdullah, M. I., Imran, M. K., & Fatima, T. (2023). When fear about health hurts performance: COVID-19 and its impact on employee's work. Review of Managerial Science, 17(2), 513-537.

ABSTRACT:

This study utilized terror management and conservation of resources theory to fulfill its aim of investigating the effects of fear of contamination of COVID-19 on performance of employees in the banking sector of Pakistan. A survey was conducted to collect data in two waves from 206 bank employees in Punjab region. SPSS was used for data analysis. The results demonstrated

that such fear leads to emotional exhaustion which in turn negatively affects employee's work performance. However, the perceptions of better precautionary measures taken by the organization against the spread of the disease moderated the said relationship and weakened the strength of fear on performance through emotional exhaustion. Amid the widespread fear, panic and detrimental effects of COVID-19 on organizations and economies of the worlds, this research has implications for policy makers by showing the importance of organizational measures taken and displayed to employees in decreasing the negative effects of extensive fear and uncertainty prevailing due to the pandemic.

Web URL: https://link.springer.com/article/10.1007/s11846-022-00536-6

10. Hasan, S., Wooliscroft, B., & Ganglmair-Wooliscroft, A. (2023). Drivers of ethical consumption: Insights from a developing country. Journal of Macromarketing, 43(2), 175-189.

ABSTRACT:
WEIRD countries (Western, Educated, Industrialised, Rich, Democratic) consume well above the earth's capacity to produce. Non-WEIRD countries look on, with justifiable envy and want to increase their standard of living. Not only do we need to reduce consumption in WEIRD countries, we need also to understand the non-WEIRD citizens' motivations to avoid/reduce future issues caused by over-consumption. This paper covers the breadth of phenomena of ethical consumption habits and their drivers in Pakistan. In-depth unstructured interviews were conducted with Pakistani respondents and analysed using laddering technique to uncover drivers of ethical consumption. Consumption choices in Pakistan are driven primarily by religiosity and frugality. While concern for health and environmental conservation is shared with WEIRD countries, underlying values (conformity and tradition) differ. These results emphasize the need to understand the drivers in developing societies and adjusting our marketing programs to improve societal wellbeing and environmental protection.

Web URL: https://journals.sagepub.com/doi/full/10.1177/02761467231168045

11. Amir, H., Bilal, K., & Khan, M. I. (2023). Efficacy of Investment in Educational Institutes and Human Capital for Sustainable Economic Growth in Pakistan. *Annals of Human and Social Sciences*, *4*(2), 586-598.

ABSTRACT:
Efficacy of investment in educational institutes, and human capital have drastic role in economic upturn. However, at various levels human capital demonstrated regarding infrastructure of education that becomes a more relevant measure of human capital alternative to enrollment at school in different institutions. This study has taken four decades annual data to investigate the association between educational institutions and human capital on economic upswing. The data starts from 1978 to 2018. The Cob Douglas production function is used to determine the efficacy of human capital, and upswing of the economy in Pakistan. The overall results reveal that there is a significant role of human capital (educational institutions) in economic growth in the long run.

It is also observed that long-term development across countries has been propelled by productivity growth at a higher scale. Economic upswing accelerates the labor productivity, if necessary, actions should be part of Government investment. The decisions, and policies in educational institutes should be positive and proof of safe flight through human capital efficacy.

Web URL: https://ojs.ahss.org.pk/journal/article/view/271

12. Gull, A. A., Abid, A., Hussainey, K., Ahsan, T., & Haque, A. (2022). Corporate governance reforms and risk disclosure quality: evidence from an emerging economy. Journal of Accounting in Emerging Economies, 13(2), 331-354.

ABSTRACT:

Purpose

The purpose of this paper is to examine the impact of corporate governance (hereafter, CG) reforms on the risk disclosure quality in an emerging economy, namely Pakistan. The authors also investigate the impact of CG reforms on the relationship between CG practices and risk disclosure quality.

Design/methodology/approach

The authors use a manual content analysis method to a sample of non-financial companies listed on the PSX-100 index for 2009–2015, to examine the impact of CG reforms on risk disclosure quality. The authors use pooled ordinary least squares and the system GMM estimations to test the research hypotheses.

Findings

The authors find that CG reforms have a positive impact on risk disclosure quality. The results indicate that certain CG practices such as CEO duality and board independence are associated with risk disclosure quality. Interestingly, the findings also highlight the effectiveness of CG reforms by showing that the revised code positively moderates the CG practices and risk disclosure relationship.

Practical implications

The findings of the study have policy implications for regulatory bodies of emerging economies trying to strengthen the CG structures and to introduce risk disclosure regulations to cater the information need of stakeholders.

Originality/value

The authors provide new empirical evidence for the impact of CG reforms on risk disclosure quality using a unique setting of an emerging economy, namely Pakistan.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/JAEE-11-2021-0378/full/html

13. Sahibzada, U. F., Jianfeng, C., Latif, K. F., Shah, S. A., & Sahibzada, H. F. (2023). Refuelling knowledge management processes towards organisational performance: mediating role of creative organisational learning. Knowledge Management Research & Practice, 21(1), 1-13.

ABSTRACT:
Constructed upon Knowledge-Based View (KBV), this research investigates the interrelationship of trust, organisational climate, Knowledge Management (KM) processes, and Organisational Performance (OP). This research further examines the intervening function of Creative Organisational Learning (COL) in an association among KM processes and OP. This research used a sample frame of 536 academic and administrative staff from research-based higher education institutes (HEI's) of China. The associations were confirmed via Smart PLS 3.2.8. The outcomes discovered that trust and organisational climate have a substantial influence on KM processes. The outcomes also reveal a direct significant impact of KM processes on OP and indirectly via COL. This unique research not only empirically examines the interface of KM enablers (trust, organisational climate), KM processes, and performance of HEI's but also enlighten visions into the present KBV literature by instantaneous investigation of the mediating role of COL.

Web URL: https://www.tandfonline.com/doi/full/10.1080/14778238.2020.1787802

14. Latif, K. F., Mas-Machuca, M., Marimon, F., & Sahibzada, U. F. (2023). Direct and configurational paths of servant leadership to career and life satisfaction in higher education: Cross-cultural study of Spain, China, and Pakistan. Journal of Human Behavior in the Social Environment, 1-24.

ABSTRACT:
This study investigates how academic staff achieves career satisfaction (CS) and life satisfaction (LS) under direct and different configurations of servant leadership (SL) dimensions. Using a survey of academics in Spain, China, and Pakistan, this study uses Partial Least Squares Structural Equation Modeling (PLS-SEM) to test the direct relationship, and fuzzy-set Qualitative Comparative Analysis (fsQCA) to find configurations of SL dimensions that lead to career and LS. Direct relationships revealed that in each country, almost all dimensions failed to create any individual impact on CS and LS. The fsQCA results revealed an asymmetric relationship between the different SL dimensions and outcomes. Prior SL, CS, and LS research has primarily relied on symmetrical correlational methods. This is one of the first studies to use fsQCA in SL, CS, and LS in higher education literature. Furthermore, there is significantly limited research on SL in a cross-country setting.

Web URL: https://www.tandfonline.com/doi/full/10.1080/10911359.2023.2218439

15. Shehzad, M. U., Zhang, J., Latif, K. F., Jamil, K., & Waseel, A. H. (2023). Do green entrepreneurial orientation and green knowledge management matter in the pursuit of ambidextrous green innovation: A moderated mediation model. Journal of Cleaner Production, 388, 135971.

ABSTRACT:

Building on the resource-based view theory, the study proposed a moderated mediation model to investigate the impact of green entrepreneurial orientation on ambidextrous green innovation (GI), the mediating role of green knowledge management, and the moderating role of resource orchestration capability. The study used a hierarchical regression analysis to examine data gathered from managers of varying levels in manufacturing firms in Pakistan. The study findings reveal that green entrepreneurial orientation influences exploitative and exploratory GIs. Green knowledge management partially mediates the relationship between green entrepreneurial orientation and exploitative and exploratory GIs. Moreover, resource orchestration capability not only strengthens the effect of green entrepreneurial orientation on green knowledge management but also the effects of green knowledge management on exploratory GI. The moderated mediation results reveal that the mediating role of green knowledge management on green entrepreneurial orientation and ambidextrous GIs is stronger when resource orchestration capability is high. These findings deepen the theoretical underpinning for green entrepreneurship, provide insight into how to enhance green innovation in manufacturing firms, and help advance the area of green entrepreneurship research.

Web URL: https://www.sciencedirect.com/science/article/pii/S0959652623001294

16. Ur Rehman, Z., Shafique, I., Khawaja, K. F., Saeed, M., & Kalyar, M. N. (2023). Linking responsible leadership with financial and environmental performance: determining mediation and moderation. International Journal of Productivity and Performance Management, 72(1), 24-46.

ABSTRACT:

Purpose

Drawing upon the institutional theory, this study examines the influence of responsible leadership on firm performance. Furthermore, this research investigates environmental management practices (EnvMP) as an underlying mechanism and institutional pressures as boundary condition between responsible leadership and firm performance.

Design/methodology/approach

Time-lagged data were collected using survey-questionnaire from 385 mid-level employees of construction industry in Pakistan. Partial least square-structural equation modeling (PLS-SEM) was used to analyze the data.

Findings

Results demonstrate that responsible leadership impacts firm performance (financial and nonfinancial) directly and through EnvMP. Furthermore, institutional pressure moderates the link between responsible leadership and EnvMP. However, moderated mediation effect of intuitional pressures was found insignificant.

Practical implications

This study suggest that EnvMP is a key process through which responsible leadership influences firms' financial and nonfinancial performance and shed lights as to when responsible leaders matter most in terms of firm performance through low or high institutional pressures.

Originality/value

This paper is an early attempt which contributes to the body of literature on responsible leadership by investigating mechanisms (how) and boundary condition (when) through which responsible leadership influences firms' financial and environmental performance.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/IJPPM-12-2020-0626/full/html

17. Shafique, I., Kalyar, M. N., Ahmad, B., & Pierscieniak, A. (2023). Moral exclusion in hospitality: testing a moderated mediation model of the relationship between perceived overqualification and knowledge-hiding behavior. International Journal of Contemporary Hospitality Management, 35(5), 1759-1778.

ABSTRACT:

Purpose

Drawing from moral exclusion theory, this study aims to examine a moderated mediation model for the relationship between perceived overqualification (POQ) and knowledge-hiding behavior directly and via perceived dissimilarity.

Design/methodology/approach

Using the convenience-sampling technique, time-lagged (three waves) data were gathered from 595 employees working in different hotels and event management firms. Hayes' PROCESS macro was used to test the moderated mediation model.

Findings

Results showed that perceived dissimilarity among coworkers mediated the result of POQ on knowledge-hiding behavior. In addition, interpersonal disliking moderated the indirect effect in a way that this effect was strong when interpersonal liking was low.

Practical implications

Findings suggest that organizations should make the overqualified realize that they can also learn from their coworkers whom they perceive as less qualified. In this, the feelings of dissimilarity and disliking can be minimized that in turn may decrease the intention to hide knowledge.

Originality/value

The present study offers a new perspective for identifying the nexus between POQ and knowledge-hiding behavior by drawing upon moral exclusion theory and examining the mediating role of perceived deep-level dissimilarity.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/IJCHM-01-2022-0067/full/html

18. Saeed, M., Adiguzel, Z., Shafique, I., Kalyar, M. N., & Abrudan, D. B. (2023). Big data analytics-enabled dynamic capabilities and firm performance: examining the roles of marketing ambidexterity and environmental dynamism. Business Process Management Journal, 29(4), 1204-1226.

ABSTRACT:

Purpose
Drawing from dynamic capability (DC) theory, this study aims to investigate how big data analytics (BDA)-enabled dynamic capabilities (DCs) prompt firm performance. This study proposes that BDA-enabled DCs lead firms toward simultaneous exploration and exploitation of new knowledge about markets and products (i.e. marketing ambidexterity) which in turn improves firms' market and financial performance. This study also examines if environmental dynamism strengthens the aforementioned relationship.
Design/methodology/approach
This study uses survey questionnaire and data were collected in the form of two heterogeneous samples from Turkey and Pakistan. Partial least square-structural equation modeling (PLS-SEM) was used to test the hypotheses.
Findings
Results reveal that BDA-enabled DCs positively affect both dimensions of marketing ambidexterity (exploration and exploitation). Marketing exploration and exploitation have positive effects on firms' market and financial performance. Results also demonstrate that environmental dynamism moderates the link between BDA-enabled DCs and firms' marketing exploitation. The moderating effect for BDA-enabled DCs and firms' marketing exploration was not consistent across both samples.
Research limitations/implications
This study contributes to the literature of BDA and marketing ambidexterity in the light of DC theory in a way that when and how the marketing ambidexterity, derived from BDA-enabled DCs, has a positive impact on firm performance. Moreover, findings imply that the development and enhancement of BDA-enabled DCs facilitate firms to calibrate marketing exploitation and exploration to seek new knowledge about markets and products and using such knowledge to achieve superior performance.
Originality/value
The novelty of present study is development of dynamic capabilities-based framework which sheds light on the role of big data for sensing, seizing and (re)configuring firms' resources to develop marketing ambidextrous capabilities in order to stay successful. From methodological perspective, this study uses two heterogeneous samples to assess robustness of results for ensuring greater generalizability and theoretical resonance.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/BPMJ-01-2023-0015/full/html

19. Kalyar, M. N., Shafique, I., Saleem, S., & Humayun, S. (2023). Role of Leadership for Blockchain-Driven Supply Chain Management. In Blockchain Driven Supply Chain Management: A Multi-dimensional Perspective (pp. 87-100). Singapore: Springer Nature Singapore.

ABSTRACT:

The emerging trends in blockchain-driven supply chain management (BCSCM) have gained popularity among practitioners in recent years. The growing scholarly interest in this discipline has unveiled various supply chain management practices; however, there is an implicit gap

concerning exploring the role of contextual factors that influence the blockchain-driven supply chain. The current chapter contributes to the literature by investigating the impact of leadership on blockchain that would radically improve supply chain management. In this chapter, we review the extant literature on the linkages among leadership, blockchain, and supply chain management. Over and above, the main objective is to understand the mechanism that how businesses may successfully introduce and integrate blockchain technology into the management of their supply networks through the role of leadership.

Web URL: https://link.springer.com/chapter/10.1007/978-981-99-0699-4_6

20. IdreesF., HassanH.,Syed T.,AhmadN., A.,KhanM., M.,(2022). Perceived Behavioral Control Mediates the Relationship between Personal Characteristics and Psycho-Sociological Factors, and Entrepreneurial Intentions

ABSTRACT:

The entrepreneurial intentionwith its antecedents is an active area of research. Perceived behavioral controlas an antecedent of entrepreneurial intentionand a mediator between the relationship of personal characteristics, psycho-sociological factors,and entrepreneurial intentions is proposed in this study.This study is grounded in the theory of reasoned action by Fishbein and Ajzen (1975), the theory of planned behavior by Ajzen (1985),and the Entrepreneurship Event Model byShapero and Sokol (1982). The datafor this study is collected from a sample survey ofthe students of higher educational institutions to empirically validate the theoretical research model. The analysis establishes that perceived behavioral controlmediates the relationship between personal characteristics, psycho-sociological factors,and EIs. The study is useful for policymakers, economists, and educationists.

Web URL: https://rjsi.org.pk/index.php/Research/article/view/50/40

21. BAKARIQBAL, M. A. (2023). ENTREPRENEURIAL PASSION AND ENTREPRENEURIAL PERFORMANCE: DUALISTIC MODEL. Russian Law Journal, 11(3).

ABSTRACT:

The fundamental objective of this paper is to produce a theoretical framework for understanding the relationship between the dualistic model of entrepreneurial passion and entrepreneurial performance. This framework draws upon the principles of the Self-Determination Theory and the Mood Maintenance Hypothesis. To gather information, a comprehensive review of existing conceptual and empirical literature on the subject was conducted, and the findings were synthesized. The results indicate that the association between dualistic model of entrepreneurial passion and entrepreneurial performance is distant. The proposed dualistic model of entrepreneurial passion directly influences entrepreneurial performance, while also exerting indirect effects that are sequentially mediated by factors such as entrepreneurial emotions, risk-taking, competitive aggressiveness, and escalation of commitment. The study presents a concise framework for regulating entrepreneurial passion and its impact on entrepreneurial performance.

It expands the ontological understanding of the dualistic model of entrepreneurial passion, and there is a high likelihood that the framework will be validated through empirical research in the future. The practical implications of this study are significant, as it offers a comprehensive understanding of the link between entrepreneurial passion and entrepreneurial performance. This studycan be utilized to develop effective strategies and interventions in the field of entrepreneurship.

Web URL: https://www.russianlawjournal.org/index.php/journal/article/view/2067

22. Shakil, M. H., Idrees, R. N., Ehsan, S., & Anwar, W. (2023). Impact of green human resource management on green creativity in pharmaceutical companies: mediation role of green mindset. Environmental Science and Pollution Research, 30(38), 88481-88494.

ABSTRACT:
This research study analyzed the impact of green human resource management on the green creativity of the employees of the pharmaceutical companies of Lahore, Pakistan, with the mediating role of a green mindset and the moderating role of green concern. The convenience sampling technique was used to sample employees of pharmaceutical companies. The study was quantitative and cross-sectional in nature, and it used correlation and regression analysis to investigate the hypothesis. A sample of 226 employees (including managers, supervisors, and other staff members) was drawn from different pharmaceutical companies in Lahore, Pakistan. The results of the study indicate that green human resource management has a positive significant effect on the green creativity of employees. Findings further explain that the green mindset acts as a mediator and partially mediates the relationship between green human resource management and green creativity. Furthermore, this study examined the role of green concern as a moderator and the results explain the insignificant relation which shows that green concern does not moderate the relationship between the green mindset and green creativity of the employees of pharmaceutical companies in Lahore, Pakistan. The practical implications of this research study are also discussed.

Web URL: https://link.springer.com/article/10.1007/s11356-023-28626-2

23. Ehsan, S., Tabasam, A. H., Ramos-Meza, C. S., Ashiq, A., Jain, V., Nazir, M. S., ... & Gohae, H. M. (2023). Does zero-leverage phenomenon improve sustainable environmental manufacturing sector: Evidence from Pakistani manufacture industry?. Global Business Review, 09721509221150876.

ABSTRACT:
The purpose of this study is to examine the key determinants of the policy of zero-leverage firms and why these firms are a financial constraint. The concept of capital structure has now adopted a new term which is known as zero-leverage (ZL) policy. Despite of endless benefits of leverage zero-leverage phenomenon is yet emerging not only just in developed countries but also in developing countries. This study has taken the sample of listed non-financial firms of Pakistan for 2006–2020. The Logit regression model is used to investigate the determinants of the zero-

leverage phenomenon. Moreover, the proxy of constraint and unconstraint firms are dividend-paying and non-dividend-paying zero-leverage firms as well as SA-index respectively. The results show that the key determinants of ZL policy are profitability, growth rate, tax and dividend. Further, findings show that most of the ZL firms are a financial constraint. However, the sub-section of ZL firms is also found financially unconstraint with high profitability.

Web URL: https://journals.sagepub.com/doi/abs/10.1177/09721509221150876

24. Li, Q., Maqsood, U. S., Zahid, R. A., & Anwar, W. (2023). Regulating CEO pay and green innovation: moderating role of social capital and government subsidy. Environmental Science and Pollution Research, 1-15.

ABSTRACT:
The Chinese government has implemented the policies to regulate executive (CEO) pay in state-owned enterprises (SOEs) with the aim of promoting wage equality. This study examines whether these policies affect the motivation of CEOs to engage in green innovation (GI). By analyzing data from Chinese listed SOEs between 2008 and 2017, the study reveals an unintended environmental consequence of regulating CEO pay. We found a negative causal relationship between regulating CEO pay and GI. Moreover, we provide evidence that social capital act as a mitigating factor promotes cooperation and a shared sense of responsibility towards sustainable practices. Additionally, government subsidies provide financial incentives and support for businesses to invest in sustainable practices and technologies, which can offset the negative impact of CEO pay regulation on GI. The results of this study offer policy recommendations to encourage sustainable environmental initiatives; the government should increase its support for GI and introduce new incentives for managers. Overall the study findings are robust and remain valid even after conducting rigorous testing with instrumental variables and other robustness checks.

Web URL: https://link.springer.com/article/10.1007/s11356-023-26641-x

25. Afridi, F. E. A., Afridi, S. A., Zahid, R. A., Khan, W., & Anwar, W. (2023). Embracing green banking as a mean of expressing green behavior in a developing economy: exploring the mediating role of green culture. Environmental Science and Pollution Research, 1-11.

ABSTRACT:
According to a plethora of research and publications, the volume and amount of pollution are largely attributable to human-made emissions. Even during the recently ended Covid-19 outbreak, there was a notable decrease in global pollution, particularly in Pakistan's heavily populated cities. Due to the current situation, it is strategically important to safeguard the environment, and there are many criteria and predictors that should be used to encourage green behavior. This study examines green banking as a means of demonstrating ecologically responsible conduct in a developing nation. A survey questionnaire was used to collect information from 280 respondents via human contact and an internet platform. Software called SmartPLS3.0 was used to analyze the structural relationships between the study's variables. The

results show that customers' adoption of green banking practices is statistically significantly influenced by their level of environmental consciousness and attitude. Similarly, green culture exhibits a substantial mediating influence between the independent variables and green behavior as well as a positive significant effect on green behavior. However, it is established that the consumer's apparent behavioral control is negligible. Particularly, the cognitive connection between behavior and culture is weak and insufficient to forecast behavior. For policymakers, especially those working in the field of green education, this study has many real-world applications.

Web URL: https://link.springer.com/article/10.1007/s11356-023-25449-z

26. Iqbal, M. Z., Shakoor, A., Ikramullah, M., & Khan, T. (2023). Do managers' negotiation styles make employees' relational justice-emotional experiences links sporadic?. International Journal of Conflict Management, 34(3), 440-467.

ABSTRACT:

Purpose

Being grounded in interdependence theory, this study aims to address the following research question: Do managers' negotiation styles (collaborative versus competitive) make employees' relational justice-emotional experiences links sporadic?

Design/methodology/approach

Data elicited from N = 139 Pakistani undergraduate students participating in an online scenario-based experiment were used to employ repeated measures analysis and partial least square structural equation modeling techniques.

Findings

Results suggest that employees' relational justice is likely to be higher when managers use a collaborative negotiation style than when they use competitive style in performance review meetings. Moreover, per managers' different negotiation styles, employees' relational justice perceptions may predict their positive emotions differently. That is, when managers use collaborative negotiation style, employees' relational justice perceptions may positively predict their hope but not optimism, whereas when managers use competitive negotiation style, employees' relational justice perceptions may positively predict their optimism but not hope. Furthermore, the positive relationship between employees' relational justice and their optimism is stronger when their trust in manager is low than when it is high.

Originality/value

The study is of value for performance management theorists who aim to address the issue of ineffectiveness of the practice through relational means. The study includes the recently explicated concept of relational justice and examines its links with employee emotional reactions to performance reviews. Moreover, the study unveils how managers' negotiation styles in performance review meetings cause variations in the links between employees' perceptions of relational justice and their emotional experiences.

Web URL: https://www.emerald.com/insight/content/doi/10.1108/IJCMA-09-2022-0150/full/html

27. Javed, Z., & Rana, M. L. T. (2022). Fostering Employees' Creativity through a Mediation Mechanism: A South Asian Perspective. Journal of Development and Social Sciences, 3(3), 635-647.

ABSTRACT:
This study aims to investigate the connection between ethical leadership and employees' creativity through affective commitment and determine whether affective commitment affects employees' creativity among workers in Punjab's telecom industry. Data from several telecom businesses in Lahore and Gujranwala were gathered using a convenience sampling technique and a self-administrated questionnaire of 284 employees. The results imply that the connection between ethical leadership and employees' creativity is mediated by affective commitment. Employees' creativity is greatly benefited by affective commitment. Additionally, the results support earlier research that suggests ethical leadership fosters creativity. The results suggest that encouraging employees' creativity requires ethical leadership and affective commitment. Strong affective commitment leads to highly innovative behavior in employees. It is advised that managers behave ethically to foster a robust affective commitment link among staff members to unleash employees' creativity.

Web URL: https://www.ojs.jdss.org.pk/journal/article/view/527

28. Javed, Z., & Rana, M. L. T. (2022). Fostering Employees' Creativity through a Mediation Mechanism: A South Asian Perspective. Journal of Development and Social Sciences, 3(3), 635-647.

ABSTRACT:
This study aims to investigate the connection between ethical leadership and employees' creativity through affective commitment and determine whether affective commitment affects employees' creativity among workers in Punjab's telecom industry. Data from several telecom businesses in Lahore and Gujranwala were gathered using a convenience sampling technique and a self-administrated questionnaire of 284 employees. The results imply that the connection between ethical leadership and employees' creativity is mediated by affective commitment. Employees' creativity is greatly benefited by affective commitment. Additionally, the results support earlier research that suggests ethical leadership fosters creativity. The results suggest that encouraging employees' creativity requires ethical leadership and affective commitment. Strong affective commitment leads to highly innovative behavior in employees. It is advised that managers behave ethically to foster a robust affective commitment link among staff members to unleash employees' creativity.

Web URL: https://www.ojs.jdss.org.pk/journal/article/view/5

29. Hou, K., Qammar, R., Zhu, C., Usman, M., & Abbas, S. (2023). Testing the resources curse hypothesis: Unleashing the role of national governance and financial development in OPEC countries. Resources Policy, 86, 104242.

ABSTRACT:
Financial development is an inclusive objective for economies worldwide, but its connection with natural resources remains a topic of debate. This study aims to address this gap by investigating the impact of the resource-curse hypothesis on economic development in Organization of the Petroleum Exporting Countries (OPEC) countries during the period 1996 to 2021, given their substantial natural resources. Employing a cross-sectional ARDL (CS-ARDL) framework and validating the cointegration results with the Pedroni, Westerlund, and Kao Co-integration tests, this research surprisingly challenges the conventional wisdom of the resource-curse hypothesis. Instead, it reveals that natural resource rents can be beneficial for promoting financial development in high-income resource-rich economies. Furthermore, the study uncovers positive associations between financial development and key factors such as government effectiveness, regulatory quality, renewable energy adoption, economic growth, and urbanization. The findings underscore the significance of strong institutional frameworks in fostering financial development and offer valuable policy recommendations to enhance financial progress in OPEC countries.

Web URL: https://www.sciencedirect.com/science/article/pii/S0301420723009534

30. Shakil, M. H., Idrees, R. N., Ehsan, S., & Anwar, W. (2023). Impact of green human resource management on green creativity in pharmaceutical companies: mediation role of green mindset. Environmental Science and Pollution Research, 30(38), 88481-88494.

ABSTRACT:
This research study analyzed the impact of green human resource management on the green creativity of the employees of the pharmaceutical companies of Lahore, Pakistan, with the mediating role of a green mindset and the moderating role of green concern. The convenience sampling technique was used to sample employees of pharmaceutical companies. The study was quantitative and cross-sectional in nature, and it used correlation and regression analysis to investigate the hypothesis. A sample of 226 employees (including managers, supervisors, and other staff members) was drawn from different pharmaceutical companies in Lahore, Pakistan. The results of the study indicate that green human resource management has a positive significant effect on the green creativity of employees. Findings further explain that the green mindset acts as a mediator and partially mediates the relationship between green human resource management and green creativity. Furthermore, this study examined the role of green concern as a moderator and the results explain the insignificant relation which shows that green concern does not moderate the relationship between the green mindset and green creativity of the employees of pharmaceutical companies in Lahore, Pakistan. The practical implications of this research study are also discussed.

Web URL: https://link.springer.com/article/10.1007/s11356-023-28626-2

31. Shakil, M. H., Idrees, R. N., Ehsan, S., & Anwar, W. (2023). Impact of green human resource management on green creativity in pharmaceutical companies: mediation role of green mindset. Environmental Science and Pollution Research, 30(38), 88481-88494.

ABSTRACT:
This research study analyzed the impact of green human resource management on the green creativity of the employees of the pharmaceutical companies of Lahore, Pakistan, with the mediating role of a green mindset and the moderating role of green concern. The convenience sampling technique was used to sample employees of pharmaceutical companies. The study was quantitative and cross-sectional in nature, and it used correlation and regression analysis to investigate the hypothesis. A sample of 226 employees (including managers, supervisors, and other staff members) was drawn from different pharmaceutical companies in Lahore, Pakistan. The results of the study indicate that green human resource management has a positive significant effect on the green creativity of employees. Findings further explain that the green mindset acts as a mediator and partially mediates the relationship between green human resource management and green creativity. Furthermore, this study examined the role of green concern as a moderator and the results explain the insignificant relation which shows that green concern does not moderate the relationship between the green mindset and green creativity of the employees of pharmaceutical companies in Lahore, Pakistan. The practical implications of this research study are also discussed.

Web URL: https://link.springer.com/article/10.1007/s11356-023-28626-2

32. Irfan, S. M., Qadeer, F., Sarfraz, M., & Bhutta, M. K. (2023). Determinants and consequences of job crafting under the boundary conditions of work uncertainty. Career Development International, 28(6/7), 686-705.

ABSTRACT:
Purpose
This paper explores critical job resources (CRJRs) as predictors of job crafting and sustainable employability. Using job demands-resources (JD-R) theory as a theoretical lens, the authors examine how job crafting mediates CRJR and sustainable employability and whether work uncertainty as a boundary condition further strengthened these associations using moderated mediation approach.
Design/methodology/approach
The authors used a cross-sectional time-lagged research design by collecting data from 483 knowledge workers in Pakistan's healthcare and universities, both public and private. The authors used structural equation modeling using AMOS 25.0 software to examine the proposed relationships' mediation, moderation and moderated-mediation processes, such as Hayes (2018) process models 1,7,14 and 58. In addition, the authors tested a structural model with self-developed estimands instead of using process macros available in SPSS by computing variables.

WebURL:https://www.emerald.com/insight/content/doi/10.1108/CDI-03-2023-0063/full/htm

33. Irfan, S. M., Qadeer, F., Sarfraz, M., & Abdullah, M. I. (2024). Relational triggers of job crafting and sustainable employability: examining a moderated mediation model. Current Psychology, 43(11), 9773-9792.

ABSTRACT:
Using the Job Demands and Resources Theory, this study examines whether relational job resources (co-worker relationship quality) trigger job crafting and sustainable employability. Further, we examine whether job crafting mediates co-worker relationship quality and sustainable employability relationships in a motivational process and to what extent work uncertainty moderates these relationships using moderated mediation approach. We tested the proposed hypothesis using a structural model and self-developed process macros for AMOS to test Hayes (2018) process models 1, 7, 14, and 58 using two-wave data of 483 knowledge workers. Results of this study indicate that co-worker relationship quality triggers job crafting and sustainable employability. Mediation results indicate co-worker relationship quality initiates a motivational process through job crafting, leading to sustainable employability as an outcome of the motivational process. Further, the relationships between co-worker support and sustainable employability mediated by job crafting are strengthened in high work uncertainty. This research adds to the work design and employability literature and addresses the three research gaps in job crafting literature regarding antecedents, consequences, and boundary conditions. Altogether results of this study show that work relationships trigger job crafting and sustainable employability, and these relationships are further strengthened in the presence of high work uncertainty.

WebURL: https://link.springer.com/article/10.1007/s12144-023-05088-w

34. Syed, T., Aslam, M. S., & Ahmad, Z. (2023). Does Relationship of Corporate Social Responsibility, Absorptive Capacity and Innovation Performance Exist in Manufacturing Micro Companies?. Research Journal for Societal Issues, 5(2), 232–252.

ABSTRACT:
This research is designed to check the Impact of kinds of Corporate Social Responsibility (CSR) on kinds of Absorptive Capacity(AC) and impact of kinds of Absorptive Capacity(AC) on Innovation performance (IP). Data was collecting from 375 employees of manufacturing micro-companies of Pakistan with the help of purposive sampling. Results indicates that there are positive impact of kinds of Corporate Social Responsibility (CSR) on kinds of Absorptive Capacity(AC). Reserch also describes that there are positive impact of kinds of Absorptive Capacity(AC) on Innovation performance (IP). The study also has managerial implications by revealing the contribution of intangible resources to innovation performance. The research also offers different configurations that production managers might choose to use to achieve innovative by using the concept of absorptive capabilities.

WebURL: https://rjsi.org.pk/index.php/Research/article/view/89

35. Shakil, M. H., Idrees, R. N., Ehsan, S., & Anwar, W. (2023). Impact of green human resource management on green creativity in pharmaceutical companies: mediation role of green mindset. Environmental Science and Pollution Research, 30(38), 88481-88494.

ABSTRACT:
This research study analyzed the impact of green human resource management on the green creativity of the employees of the pharmaceutical companies of Lahore, Pakistan, with the mediating role of a green mindset and the moderating role of green concern. The convenience sampling technique was used to sample employees of pharmaceutical companies. The study was quantitative and cross-sectional in nature, and it used correlation and regression analysis to investigate the hypothesis. A sample of 226 employees (including managers, supervisors, and other staff members) was drawn from different pharmaceutical companies in Lahore, Pakistan. The results of the study indicate that green human resource management has a positive significant effect on the green creativity of employees. Findings further explain that the green mindset acts as a mediator and partially mediates the relationship between green human resource management and green creativity. Furthermore, this study examined the role of green concern as a moderator and the results explain the insignificant relation which shows that green concern does not moderate the relationship between the green mindset and green creativity of the employees of pharmaceutical companies in Lahore, Pakistan. The practical implications of this research study are also discussed.

WebURL: https://link.springer.com/article/10.1007/s11356-023-28626-2

36. Qammar, A., Sagheer, R., & Aslam, M. S. (2024). Translating environmental corporate social responsibility into environmental performance and competitive advantage: a moderated mediation model. Environmental Science and Pollution Research, 31(34), 46293-46311.

ABSTRACT:
Abstract
Organizations are extending their corporate social responsibility (CSR) practices to environmental corporate social responsibility (ECSR) to cope with environmental challenges. Yet, the process of translating ECSR into positive organizational outcomes is underdeveloped in the literature. The literature often ignored key boundary conditions, leaving the underlying mechanism underdeveloped. This research makes up for the deficiency by investigating the impact of ECSR on environmental performance and competitive advantage through the mediation of green product innovation and by examining important boundary conditions in a moderated mediation model. We collected data from 151 manufacturing companies using judgmental and snowball sampling to ensure that the target organizations perform certain ECSR activities and analyzed it using partial least square structural equation modelling (PLS-SEM). The findings reveal that ECSR leads to competitive advantage (CA) and environmental performance (EP) through green product innovation, and this indirect path is moderated by organizational agility. The findings add substantial value to the literature by documenting the impact of ECSR on CA and EP with moderated mediation paths. The study also offers implications for policymakers and managers to amplify the impact of ECSR on favorable organizational outcomes.

WebURL: https://link.springer.com/article/10.1007/s11356-023-29689-x

37. Sarwar, A., Abdullah, M. I., Imran, M. K., & Rafiq, N. (2023). How ostracism jeopardizes customers' interests at restaurants: a study in context of COVID-19. Journal of Asian Business and Economic Studies, 30(3), 210-225.

ABSTRACT:

Purpose

With theoretical underpinnings in the conservation of resources theory, this research aims at understanding the link between workplace ostracism (WPO) and its effects on customers' interests in the context of COVID-19, with the mediation of stress and moderation of self-efficacy (SE).

Design/methodology/approach

The study followed a time-lagged design. A sample of 217 frontline employees working in the food sector of southern Punjab, Pakistan, responded to the study questions using the survey method with structured questionnaires. A Statistical Package for the Social Sciences (SPSS) tool was utilized for data analysis with bootstrapping and PROCESS macro.

WebURL:https://www.emerald.com/insight/content/doi/10.1108/JABES-12-2021-0215/full/html

38. Gull, A. A., Abid, A., Nguyen, D. K., Usman, M., & Mushtaq, R. (2024). Stock price crash and information environment: Do CEO gender and financial expertise matter?. Review of Quantitative Finance and Accounting, 1-37.

ABSTRACT:

This study examines the effect of stock price crash on the information environment. We further investigate the effect of female and financial expert CEOs on the stock price crash and information environment nexus. Employing one of the largest datasets to-date of Chinese A-share listed firms (i.e., over 35,000 firm-year observations), our findings are twofold. First, consistent with agency and information asymmetry perspective, we find that stock price crash deteriorates the quality of information environment. Second, consistent with resource dependence view, our findings reveal that the presence of female and financial expert CEOs mitigate the stock price crash and information environment relationship. Our findings are robust to different endogeneity tests (e.g., two-stage least squares, propensity score matching, bootstrapping, and the system generalized method of moments), alternate proxies and additional analyses. This study contributes to the literature on portfolio investment and risk management.

WebURL: https://link.springer.com/article/10.1007/s11156-024-01244-w

39. Usman, M., Umar, Z., Choi, S. Y., & Teplova, T. (2024). Quantifying endogenous and exogenous shocks to financial sector systemic risk: A comparison of GFC and COVID-19. The Quarterly Review of Economics and Finance, 94, 281-293.

ABSTRACT:
In this study, we use segregated endogenous and exogenous shocks to large banks' returns to compare the effect of each on financial sector systemic risk. We use the copula-CoVaR methodology and GARCH (1,1) with time-varying moments to model the marginal distribution function and bivariate probability distribution of the tail returns. We find that endogenous risk dominates exogenous risk in the financial system. A comparison of the 2008 global financial crisis and COVID-19 reveals that the crisis aggravates only as exogenous shocks to the system persist. Additionally, we find that large banks reduce the total risk of the system in normal times but increase the risk of the financial system in crisis times. Our findings have important implications for policymakers, investors, and portfolio managers.
WebURL: https://www.sciencedirect.com/science/article/pii/S1062976924000218

40. Umar, Z., Hadhri, S., Abakah, E. J. A., Usman, M., & Umar, M. (2024). Return and volatility spillovers among oil price shocks and international green bond markets. Research in International Business and Finance, 69, 102254.

ABSTRACT:
We analyse the spillover effects between oil price shocks and green bonds issued in twelve developed economies. We decompose oil price shocks into demand, risk and supply shocks. We employ daily data from December 2008 to June 2022 enabling us to cover major global crisis episodes such as the global financial crisis, European sovereign debt crisis, Covid-19 pandemic, Russia-Ukraine conflict, and the corresponding boom and bust in energy markets. Our results show the dominance of the US and the European green bond markets as the main contributors to return and volatility spillovers among international green bonds, respectively. The degree of connectedness among markets varies over time with a more pronounced effect on returns during turbulent periods. Oil shocks exhibit a relatively low degree of connectedness with green bonds implying potential diversification attributes. This result is, particularly, supported in the case of green bond markets of USA, Euro, Denmark and Hong-Kong.

WebURL: https://www.sciencedirect.com/science/article/pii/S0275531924000461

41. Anwar, A., Rashid, M. A., Irfan, S. M., & Hussain, G. Effect of Perceived Negative Workplace Gossip on Trickle-Down Effect of Knowledge-Hiding within the Organizations.

ABSTRACT:
Knowledge hiding has emerged as a real challenge in today's knowledge economies, curbing an organization's ability to attain sustainable growth and adversely affecting individuals and organizational culture, performance, and retaining talent. This study explores the effect of perceived negative workplace gossip (PNWG) on supervisors' knowledge-hiding (SKH) behavior and how supervisors' knowledgehiding behavior trickles down into the behaviors of subordinates. Based on the conservation of the resource and social cognition as a theoretical lens, this study examines the relationship between PNWG, SKH, and subordinates' knowledge-hiding from co-workers (SKHC) with a mediating role of subordinates' moral disengagement (MD) using a multilevel approach. Data were collected from 108 supervisors and 492 subordinates of employees of small and medium enterprises (SMEs). Mplus software was used to analyze the multilevel relationships. The results of this study reveal that PNWG influences SKH; SKH is positively associated with SKHC; finally, we found that MD mediates the relationship between SKH and SKHC. This study brings

new insights by uncovering the relationships between the studied variables using a multilevel approach and the underexplored trickle-down effects of knowledge-hiding in SMEs. This study has important theoretical implications and practical suggestions for organizations and human resources managers to develop policies and procedures to overcome this issue and make organizations and individuals more productive and valuable.

WebURL: https://www.sciencedirect.com/science/article/pii/S0275531924000461

42. Chohan, A., Hussain, G., & Shafique, I. (2024). Does social capital affect supply chain performance? Establishing an underlying mechanism and a boundary condition. International Journal of Productivity and Performance Management.

ABSTRACT:

This study examines the direct and indirect effects of social capital on supply chain performance via supply chain quality integration (SCQI), which refers to integrating supply chain partners from the perspective of quality management. It also examines the moderating role of environmental uncertainty in the link between social capital and SCQI and determines the conditional indirect effect of social capital on supply chain performance via SCQI.

Design/methodology/approach

Data were collected using a time-lagged research design through a self-administered survey of supply chain professionals in manufacturing firms in Pakistan. Hayes' PROCESS Macro was used to test the hypotheses.

Findings

The results show a positive relationship between social capital and supply chain performance. SCQI partially mediates the relationship between social capital and supply chain performance. Environmental uncertainty significantly moderates that relationship in such a way that firms that operate under high environmental uncertainty are more likely to use their social capital to develop SCQI than firms that operate under low environmental uncertainty.

Practical implications

The study has practical implications for managers who seek to implement SCQI practices using social capital. Leveraging social capital across the supply chain fosters strong connections and a quality-oriented approach across the supply chain, and improves overall performance. Managers can use the power of social capital to navigate environmental uncertainty.

Originality/value

This study's originality lies in its drawing on the dynamic capability theory and contingency theory and integrating the dispersed scholarly work on social capital, SCQI, and supply chain performance under the boundary condition of environmental uncertainty.

WebURL:https://www.emerald.com/insight/content/doi/10.1108/IJPPM-06-2023-0291/full/html

43. Hussain, G., Samreen, F., Riaz, A., Wan Ismail, W. K., & Sultan, M. (2024). A cross-level relationship between entrepreneurial leadership and followers' entrepreneurial intentions through entrepreneurial self-efficacy and identification with the leader under moderating role of cultural values. Current Psychology, 43(8), 7478-7496.

ABSTRACT:

Grounded in Social Cognitive Theory, this study examines entrepreneurial self-efficacy and identification with the leader as mediating mechanisms that account for the cross-level relationship between entrepreneurial leadership and entrepreneurial intentions. This study also establishes the moderating role of (a) individualism between entrepreneurial leadership and entrepreneurial intentions, and (b) collectivism between entrepreneurial leadership and personal identification with the leader. We collected data through self-administered questionnaires from IT professionals working in small and medium-sized IT solution provider firms. To enhance the generalizability, samples were selected from China (n = 234) and Pakistan (n = 209). Further, a multi-level research design was used for analysis. The results showed that entrepreneurial leadership has a significant positive relationship with entrepreneurial intentions. The results for the mediating effects showed that entrepreneurial self-efficacy and identification with the leader significantly mediated between entrepreneurial leadership and entrepreneurial intentions. The moderating effects results supported the moderating effects of (a) individualism on entrepreneurial leadership and entrepreneurial self-efficacy, and (b) collectivism on entrepreneurial leadership and personal identification with the leader. The conditional indirect effects of entrepreneurial leadership on entrepreneurial intentions via entrepreneurial self-efficacy and identification with the leader were high at high individualism and high collectivism, respectively. This study, for the first time, establishes relationships between entrepreneurial leadership and entrepreneurial intentions in Asian economies. Our study complements and extends the entrepreneurship and leadership literature in developing countries' contexts.

WebURL: https://link.springer.com/article/10.1007/s12144-023-04935-0

44. Shakil, M. H., Mukarram, M., Hussain, G., Idrees, R. N., & Sajjad, A. (2024). The influence of green human resource management on environmental performance: An empirical study investigated in the pollutant industries of Pakistan. Business Strategy & Development, 7(1), e313.

ABSTRACT:

This research mainly aims to test the impact of green human resource management (GHRM) on environmental performance (EP) and to determine whether corporate social responsibility (CSR) mediates the relationship between GHRM and EP and whether organizational citizenship behavior (OCB) moderates the relationships between CSR and EP. The paper relied on a quantitative research approach with a sample of 204 employees from the pollutant industries of Pakistan. In this paper, the partial least square approach (PLS-SEM) was employed to verify the proposed hypotheses. The outcomes confirmed that GHRM has a positive impact on EP. Additionally, the findings indicated that CSR affected EP. It was also revealed that CSR fully mediates the linkages between GHRM and EP. This paper acknowledges the existing gaps in the prior literature and enables us to clearly understand the significance of GHRM in affecting EP via CSR as a mediator.

WebURL: https://onlinelibrary.wiley.com/doi/full/10.1002/bsd2.313

45. Ali, M., Usman, M., Khan, M. A. S., Shafique, I., & Mughal, F. (2024). "Articulating cognizance about what to hide what not": Insights into why and when ethical leadership

regulates employee knowledge-hiding behaviors. Journal of Business Ethics, 190(4), 885-895.

ABSTRACT:
Given the dearth of research examining the distinctions across various facets of employee knowledge-hiding (KH) behaviors, there is little known about why and when leadership negatively influences playing dumb and evasive hiding but positively influences rationalized hiding. The present study fills this void by hypothesizing that employee justice orientation (JO) acts as a mediator of the associations of ethical leadership (EL) with different facets of employee KH behaviors. We also propose employee conscientiousness moderates the relationship of EL with JO and the indirect relationships of ethical leadership with distinct variants of employee KH behaviors. The results based on time-lagged data from 387 employees provide support for the hypothesized relationships. Together, our research provides a more nuanced account of the influence of leadership on employee KH behaviors that can facilitate the development of more appropriate interventions to deal with the intricate problems related to employee KH behaviors.

WebURL: https://link.springer.com/article/10.1007/s10551-023-05426-9

46. Aslam, M. S., & Akram, A. (2024). When and how does e-HRM optimize communication pace and processing time?. Journal of Economic and Administrative Sciences.

ABSTRACT:
This study aims investigate the effects of electronic human resource management (e-HRM) on communication pace and processing time reduction through the mediation of organizational agility. The study also investigates the moderating role of technological attitude (TA) on the relationship between e-HRM and organizational agility.
Design/methodology/approach
The data was collected from 331 information and communication technology (ICT) companies – one respondent from each company working in the Human Resource Management (HRM) department. The data was analyzed through the partial least square structural equational model (PLS-SEM) using WarpPLS7.0 software to test the study's hypotheses.
Findings
We found that e-HRM has positive significant effects on communication pace and processing time reduction through the mediation of organizational agility. Furthermore, TA is found to be positively moderating the relationship between e-HRM and organizational agility.
Research limitations/implications
The study adds significant value to the existing knowledge base on e-HRM by providing empirical insights about the role of e-HRM in optimizing the communication pace and processing time of today's businesses.
Practical implications
The study also provides invaluable insights to practitioners to replace conventional HR systems with e-HRM to better perform HR functions by optimizing communication pace and processing time in the current fast-paced era.
Originality/value

E-HRM has become an issue of great significance in the contemporary corporate landscape to improve operational efficiency. Despite its widespread adoption in the corporate world, empirical evidence on e-HRM, particularly on its consequences, is still inconclusive.
WebURL:https://www.emerald.com/insight/content/doi/10.1108/JEAS-01-2024-0037/full/html

47. Aslam, M. S., Qammar, A., Ali, I., Yaqub, M. Z., Ahmed, F., & Mohapatra, A. K. (2024). Fostering innovation speed and quality in ICT firms: The role of knowledge governance mechanisms, absorptive capacity and environmental dynamism. Technological Forecasting and Social Change, 205, 123460.

ABSTRACT:
While considerable research has probed into the dynamics of innovation through knowledge management, significant gaps persist. The current study addresses these gaps by exploring the impact of formal and informal knowledge governance mechanisms (KGMs) on innovation speed and quality through the mediation of absorptive capacity. In addition, the moderating role of environmental dynamism in the interplay between absorptive capacity and innovation speed and quality is also examined. Data for this two-wave time-lagged study is collected in a survey from 331 managerial employees working in different organizations in the Information Communication and Technology (ICT) sector. Using WarpPLS 7.0 for statistical analysis, the study found that formal and informal KGMs have a positive significant relationship with innovation speed and quality through the mediation of absorptive capacity. Further, environmental dynamism positively moderates the relationship between absorptive capacity and innovation speed and quality. The findings contribute by enhancing our understanding of the role of KGMs in fostering innovation speed and quality, providing actionable insights for organizations to improve their innovation strategies.

WebURL: https://www.sciencedirect.com/science/article/pii/S0040162524002567

DEPARTMENT OF MATHEMATICS

1. Saleem, R., Ali, S., & Aslam, M. I. (2023). Dynamical study of NTADE and SMHDE models within Rastall gravity. Chinese Journal of Physics, 81, 78-91.

ABSTRACT:
This paper is mainly focused to investigate the cosmological implications of Rastall gravity with the help of two dark energy models, i.e., new Tsallis agegraphic dark energy (NTADE) and Sharma–Mittal holographic dark energy (SMHDE). The background of flat FLRW space–time is being considered to develop the dynamical system of equations. To check the viability of these models and to distinguish them, we develop some important cosmological parameters. By constraining the involved model parameters, it is observed that the equation of state (EoS) parameter for the NTADE model lies in the phantom region whereas, for SMHDE, it shows quintom as well as quintessence regions depending on the values of model parameter δ. The deceleration parameter shows the phase transition from decelerating to the accelerating phase for both models. The $\omega D - \omega\ ' D$ pair shows freezing and thawing regions for NTADE, and the freezing region for SMHDE. The pair (j, s) for SMHDE indicates a rich behavior as it shows different DE eras, a phantom, the quintessence as well as Chaplygin gas but the NTADE model shows Chaplygin gas behavior only. We conclude that SMHDE is a more efficient model than the NTADE model because it approaches ΛCDM limit and the results for this model lie in a stable region as shown by graphical analysis of the square speed of sound.

Web URL: https://www.sciencedirect.com/science/article/pii/S0577907322002799

2. Faisal Nadeem, M., & Azeem, M. (2023). The fault-tolerant beacon set of hexagonal Möbius ladder network. Mathematical Methods in the Applied Sciences, 46(9), 9887-9901.

ABSTRACT:
In localization, some specific nodes (beacon set) are selected to locate all nodes ofa network, and if an arbitrary node stops working and still selected nodes remainin the beacon set, then the chosen nodes are called fault-tolerant beacon set.Due to the variety of metric dimension applications in different areas of sciences,many generalizations were proposed, fault-tolerant metric dimension is one ofthem. A resolving (beacon) setB$f$is fault tolerant, ifB$f\backslash v$for each$v\in$B$f$isalso a resolving set; it is also known as a fault-tolerant beacon set; the minimumcardinality of such a beacon set is known as the fault-tolerant metric dimensionof a graphG. In this paper, we find the fault-tolerant beacon set of hexagonalMöbius ladder networkH(α,β)and proved that all the different variations ofαandβinH(α,β)has constant fault-tolerant metric dimension

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/mma.9091

3. Saleem, R., Aslam, M. I., & Rasool, K. (2023). Wormhole solutions in Rastall-like-torsion-trace gravity. Chinese Journal of Physics, 82, 1-14.

ABSTRACT:
In this paper, we explore the existence of traversable wormholes (WHs) inspired by the non-commutative (NC) geometry under conformal symmetries in the framework of Rastalllike-teleparallel gravity. Using ‘‘Gaussian’’ and ‘‘Lorentzian’’ energy distributions, we calculate the analytic solutions of the corresponding field equations in terms of some special math functions. For both distributions, we check the viability of energy conditions at the WH throat and interpret the results graphically for appropriate choices of free model parameters along with different choices of additional Rastall parameter λ. We explain the possible constraints for the positivity of active gravitational mass, and check the stability of derived WH solutions. Moreover, the embedding diagrams for the shape functions are also plotted. Finally, it is concluded that the constructed WH solutions (sensitive for parameter λ) are physically viable as well as stable in the presence of standard matter for Gaussian energy distribution and exotic matter for Lorentzian energy distribution.

Web URL: https://www.sciencedirect.com/science/article/pii/S0577907322003070

4. M. Ghazanfar Monir , M. Rafiullah , Faiza Waqqas , Habib Shaukat. Implementation and analysis of symmetrical signals in the sequence domain

ABSTRACT:
Every transform has unique attributes and traits that are crucial to reducing computing costs and offering simple solutions. Many different frequency domain transformations, for instance, have properties that can be used in a variety of signal processing applications and analyses. Some of the Complex Hadamard Transform's variants' sequencies can be compared to those of the Discrete Fourier Transforms. It is proven the characteristics of the Conjugate Symmetric Sequency-Ordered Complex Hadamard Transform symmetry. These qualities are crucial for signal analysis and image processing. Due to duplicate spectra across the origin, it reduces computational complexity, makes an analytical analysis for symmetric signals simpler, and needs less storage. Its analysis shows that the Discrete Fourier Transform and this Complex Hadamard Transform version exhibit similar symmetry tendencies. By using elementary signals in the time domain to connect the positive and negative sequencies with their associated phasor conceptions, sequency domain spectra are used to highlight these properties. As a result of image representation, relative spectra are represented in related domains. Transform can be used to extract and analyze various aspects from a wide range of medical images.

Web URL: Implementation and analysis of symmetrical signals in the sequency domain (science-gate.com)

5. Shahid, I., Saleem, R., & Kausar, H. R. (2023). Warm inflation in hybrid metric-Palatini gravity under standard and irreversible thermodynamical approach. The European Physical Journal C, 83(1), 1-11.

ABSTRACT:
The idea of hybrid metric-Palatini f (X) gravity (HMPG) is a blend of Einstein Hilbert (EH) action having non-linear function f (R) and linear scalar curvature R by Palatini gravity. The goal of this paper is to investigate the warm inflationary model (WIM) via standard and irreversible thermodynamical approach in f (X) gravity. We start our work by obtaining the field equations (FEs) for HMPG and then investigate the cosmic inflation in f (X) theory of gravity by looking at cosmic parameters such as slow-roll parameters, spectral index (ns), running of spectral index (αs) and tensor-to-scalar ratio (r). Next, the early universe is considered as an open system. The thermodynamics and dynamical equations in f (X) gravity are applied to interacting cosmic fluid, which leads us to adapt the basic formalism of WIM. This analysis is done using Higgs Potential (HP). Numerical results of the thermodynamical equations such as scale factor (a(t)), scalar-field energy density (ρϕ) and radiation energy density (ργ), number of scalar-field particles (nϕ) and temperature (T) are derived and presented graphically using slow-roll approach and defining several dimensionless variables. From obtained results, we calculate cosmic parameters. In the end, we constraint the model parameters, and compare our calculated results to the Planck-2018 data

Web URL: https://link.springer.com/article/10.1140/epjc/s10052-023-11200-y

6. Qi, H., Saleem, M. S., Ahmed, I., Sajid, S., & Nazeer, W. (2023). Fractional version of Ostrowski-type inequalities for strongly p-convex stochastic processes via ak-fractional Hilfer–Katugampola derivative. Journal of Inequalities and Applications, 2023(1), 12.

ABSTRACT:
The idea of hybrid metric-Palatini f (X) gravity (HMPG) is a blend of Einstein Hilbert (EH) action having non-linear function f (R) and linear scalar curvature R by Palatini gravity. The goal of this paper is to investigate the warm inflationary model (WIM) via standard and irreversible thermodynamical approach in f (X) gravity. We start our work by obtaining the field equations (FEs) for HMPG and then investigate the cosmic inflation in f (X) theory of gravity by looking at cosmic parameters such as slow-roll parameters, spectral index (ns), running of spectral index (αs) and tensor-to-scalar ratio (r). Next, the early universe is considered as an open system. The thermodynamics and dynamical equations in f (X) gravity are applied to interacting cosmic fluid, which leads us to adapt the basic formalism of WIM. This analysis is done using Higgs Potential (HP). Numerical results of the thermodynamical equations such as scale factor (a(t)), scalar-field energy density (ρϕ) and radiation energy density (ργ), number of scalar-field particles (nϕ) and temperature (T) are derived and presented graphically using slow-roll approach and defining several dimensionless variables. From obtained results, we calculate

cosmic parameters. In the end, we constraint the model parameters, and compare our calculated results to the Planck-2018 data

Web URL: https://link.springer.com/article/10.1186/s13660-022-02901-1

7. Kiran Naz ·Sarfraz Ahmad· Muhammad Kamran Siddiqui· Hafiz Muhammad Bilal· Muhammad Imran. On Computing Some Degree Based Topological Indices for Polythiophene Networks

ABSTRACT:
Chemical graph theory is the field which deals with the combination of chemistry and graph theory. In this paper, we find the degree based first and second K Bbanhatti, first and second hyper K Banhatti, first and second multiplicative K banhatti, first and second multiplicative hyper K banhatti, Sombor, K G , modified K G , multiplicative K G , multiplicative modified K G , K Harmonic and multiplicative K Harmonic Banhatti, first Banhatti and reduced Banhatti Sombor, delta Banhatti Sombor indices for backbone DNA and subdivided backbone DNA networks. These topological descriptors are computed by direct method.
Chemical graph theory is the field which deals with the combination of chemistry and graph theory. In this paper, we find the degree based first and second K Bbanhatti, first and second hyper K Banhatti, first and second multiplicative K banhatti, first and second multiplicative hyper K banhatti, Sombor, KG, modified KG, multiplicative KG, multiplicative modified KG, K Harmonic and multiplicative K Harmonic Banhatti, first Banhatti and reduced Banhatti Sombor, delta Banhatti Sombor indices for backbone DNA and subdivided backbone DNA networks. These topological descriptors are computed by direct method.

Web URL: (PDF) On computing some degree based topological indices for backbone DNA networks (researchgate.net)

8. Rizvi, S. T., Seadawy, A. R., Nimra, & Ahmad, A. (2023). Study of lump, rogue, multi, M shaped, periodic cross kink, breather lump, kink-cross rational waves and other interactions to the Kraenkel–Manna–Merle system in a saturated ferromagnetic material. Optical and Quantum Electronics, 55(9), 813.

ABSTRACT:
The analytical rational solitons of the Kraenkel–Manna–Merle (KMM) system in a saturated ferromagnetic material will be explored in depth by using the symbolic computation with ansatz functions and logarithmic transformation. We investigate many systematic solutions such as lump soliton, rogue wave, lump with one kink, multiwave, periodic wave, periodic cross-kink wave and breather lump wave. We also examine M-shaped rational solution, homoclinic breather solution, M-shaped rational solution with one kink, kink-cross rational solution and M-shaped rational solution with two kink for KMM system. Additionally, we will draw graphs in different

dimensions allowing analytical approaches to identify the structure of enormous waves. Furthermore, we look into the stability of a derived solutions and give a results in a tables.

Web URL: https://link.springer.com/article/10.1007/s11082-023-04972-w

9. Shah, S. G. A., Al-Sa'di, S. U., Hussain, S., Tasleem, A., Rasheed, A., Cheema, I. Z., & Darus, M. (2023). Fekete-Szegö functional for a class of non-Bazilevic functions related to quasi-subordination. Demonstratio Mathematica, 56(1), 20220232.

ABSTRACT:
In this article, we study the Fekete-Szegö functional associated with a new class of analytic functions related to the class of bounded turning by using the principle of quasi-subordination. We derived the coefficient estimates including the classical Fekete-Szegö inequality for functions belonging to this class. We also improved some existing results.

Web URL: https://www.degruyter.com/document/doi/10.1515/dema-2022-0232/html

10. Zeng, X. X., Aslam, M. I., & Saleem, R. (2023). The optical appearance of charged four-dimensional Gauss–Bonnet black hole with strings cloud and non-commutative geometry surrounded by various accretions profiles. The European Physical Journal C, 83(2), 129.

ABSTRACT:
Thanks for the releasing image of supermassive black holes (BHs) by the event horizon telescope (EHT) at the heart of the M87 galaxy. After the discovery of this mysterious object, scientists paid attention to exploring the BH shadow features under different gravitational backgrounds. In this scenario, we study the light rings and observational properties of BH shadow surrounded by different accretion flow models and then investigate the effect of model parameters on the observational display and space-time structure of BHs in the framework of our considering system. Under the incompatible configuration of the emission profiles, the images of BHs comprise that the observed luminosity is mainly determined by direct emission, while the lensing ring will provide a small contribution of the total observed flux and the photon ring makes a negligible contribution due to its exponential narrowness. More importantly, the observed regions and specific intensities of all emission profiles are changed correspondingly under variations of parameters. For optically thin accreting matters, we analyze the profile and specific intensity of the shadows with static and infalling accretions models, respectively. We find that with an infalling motion the interior region of the shadows will be darker than the static case, due to the Doppler effect of the infalling movement. Finally, it is concluded that these findings support the fact that the change of BH state parameters will change the way of space-time geometry, thus affecting the BH shadow dynamics.

Web URL: https://link.springer.com/article/10.1140/epjc/s10052-023-11274-8

11. Rizvi, S. T., Seadawy, A. R., Bashir, A., & Nimra. (2023). Lie symmetry analysis and conservation laws with soliton solutions to a nonlinear model related to chains of atoms. Optical and Quantum Electronics, 55(9), 762.

ABSTRACT:
We present the Lie symmetry analysis for the famous nonlinear equation describing chains of atoms with long range interaction. We also study the conservation laws by computing the conserved density and their associated fluxes by applying the scaling invariance approach. We use the Euler and the homotopy operators for the computations of conserved density and their corresponding fluxes respectively. In addition to these, we use an auxiliary ordinary differential equation method namely sub-ODE scheme to obtain bell type, kink shape, Jacobi elliptic, hyperbolic and few other solitary wave solutions with some constraints. At the end, we discuss our results graphically in distinct dimensions.

Web URL: https://link.springer.com/article/10.1007/s11082-023-05049-4

12. Arshad, S., Saleem, I., Akgül, A., Huang, J., Tang, Y., & Eldin, S. M. (2023). A novel numerical method for solving the Caputo-Fabrizio fractional differential equation. AIMS Math, 8, 9535-9556.

ABSTRACT:
In this paper, a unique and novel numerical approach—the fractional-order Caputo-Fabrizio derivative in the Caputo sense—is developed for the solution of fractional differential equations with a non-singular kernel. After converting the differential equation into its corresponding fractional integral equation, we used Simpson's 1/3 rule to estimate the fractional integral equation. A thorough study is then conducted to determine the convergence and stability of the suggested method. We undertake numerical experiments to corroborate our theoretical findings.

Web URL: https://www.aimspress.com/aimspress-data/math/2023/4/PDF/math-08-04-481.pdf

13. Rizvi, S. T., Seadawy, A. R., & Nimra. (2023). Discussion on Peyrard Bishop DNA model for multi and breather waves, M-shaped rational and other interactional solutions. Optical and Quantum Electronics, 55(8), 670.

ABSTRACT:
In this article, we explore analytical rational solutions to the Peyrard Bishop DNA (PB-DNA) model such as lump soliton, kink soliton, periodic cross kink, multi wave and breather lump wave. By using ansatz transformation, we explore M-shaped rational solution for PB-DNA equation. Also, we acquire M-shaped rational solution with one kink and two kink. Furthermore, we compute kink cross rational solution, homoclinic breather solution. Additionally, two forms of interactions between the kinks waves and M-shaped rational solutions will be computed.

Consequently, we study the stability of the acquired solutions and present in the form of table. We also illustrate our graphs in different dimensions such as 3D, 2D, contour and stream plots.

Web URL: **https://link.springer.com/article/10.1007/s11082-023-04812-x**

14. Ama-Tul-Mughani, Q., Saleem, R., Salam, W. U., & Sadiq, S. (2023). Criticality and phase transition of Kerr–anti-de Sitter black hole with quintessence and cloud of strings. Astroparticle Physics, 148, 102820.

ABSTRACT:
In this paper, a thermodynamical study of the Kerr–anti-de Sitter (KAdS) black hole (BH) encircled by quintessence matter and the cloud of strings is presented. We check the effects of the cloud parameter on the thermodynamical variables including Hawking temperature, entropy, Helmholtz free energy (HFE), Gibbs free energy (GFE), and specific heat capacity. These thermodynamic variables hold the Smarr–Gibbs–Dehum (SGD) relation in the appearance of quintessence and the cloud of the string parameter. Then we calculate the critical expressions of the developed variables in two different ways that are "Van-der-Waals (vdW)-type equation of state" (EoS) and the "Maxwell equal-area law" (MEAL). The latter technique is found to be more reasonable to examine the criticality of the complex BHs. Using MEAL, we plot the phase diagram in a temperature–entropy plane and obtain an isobar, which represents the co-existence region of liquid–gas phases. It is concluded that the uncharged BHs exhibit the same phase transition (PT) to vdW fluid as the temperature drops down its critical value. Also, we discuss the influence of thermal fluctuations (TF) on the stability of KAdS BH.

Web URL: **https://www.sciencedirect.com/science/article/pii/S0927650523000063**

15. Saleem, R., & Aslam, M. I. (2023). Observable features of charged Kiselev black hole with non-commutative geometry under various accretion flow. The European Physical Journal C, 83(3), 1-14.

ABSTRACT:
The light passing near the black hole (BH) is deflected due to the gravitational effect, producing the BH shadow, a dark inner region that is often surrounded by a bright ring, whose optical appearance comes directly from BH's mass and its angular momentum. We mainly study the shadow and observable features of non-commutative (NC) charged Kiselev BH, surrounded by various profiles of accretions. To obtain the BH shadow profile, we choose specific values of the model parameters and concluded that the variations of each parameter directly vary the light trajectories and size of BH. For thin disk accretion, which includes direct lensing and photon rings emissions, we analyze that the profile of BH contains the dark interior region and bright photon ring. However, their details depends upon the emissions, generally, direct emission plays significant role in the total observed luminosity, while lensing ring has a small contribution and the photon ring makes a negligible contribution, as usual, the latter can be ignored safely. Moreover, we also consider the static and infalling accretion matters and found that the location

of the photon sphere is almost the same for both cases. However, the specific intensity which is observed from BH profile found to be darker for infalling accretion case due to the Doppler effect of the infalling motion as compared to the static one.

Web URL: https://link.springer.com/article/10.1140/epjc/s10052-023-11418-w?utm_medium=cpc&utm_source=trendmd&utm_content=paid&utm_term=null&utm_campaign=MPSR_OAJRN_AWA1_GL_MPAS_01WN0_CONTI-TMD_Springer

16. Sadia Arshad , Imran Siddique , Fariha Nawaz, Aqila Shaheen, Hina Khurshid. Dynamics of a fractional order mathematical model for COVID-19 epidemic transmission

ABSTRACT:
To achieve the aim of immediately halting spread of COVID-19 it is essential to know the dynamic behavior of the virus of intensive level of replication. Simply analyzing experimental data to learn about this disease consumes a lot of effort and cost. Mathematical models may be able to assist in this regard. Through integrating the mathematical frameworks with the accessible disease data it will be useful and outlay to comprehend the primary components involved in the spreading of COVID-19. There are so many techniques to formulate the impact of disease on the population mathematically, including deterministic modeling, stochastic modeling or fractional order modeling etc. Fractional derivative modeling is one of the essential techniques for analyzing real-world issues and making accurate assessments of situations. In this paper, a fractional order epidemic model that represents the transmission of COVID-19 using seven compartments of population susceptible, exposed, infective, recovered, the quarantine population, recovered–exposed, and dead population is provided. The fractional order derivative is considered in the Caputo sense. In order to determine the epidemic forecast and persistence, we calculate the reproduction number R0. Applying fixed point theory, the existence and uniqueness of the solutions of fractional order derivative have been studied . Moreover, we implement the generalized Adams–Bashforth–Moulton method to get an approximate solution of the fractional-order COVID-19 model. Finally, numerical result and an outstanding graphic simulation are presented

Web URL: https://www.sciencedirect.com/science/article/pii/S0378437122009414

17. R Saleem and Aqsa Saleem. Baryogenesis inspired by some modified entropies. 2023 *Phys. Scr.* **98 055021**

ABSTRACT:
Entropy is defined as a measure of the degree of disorder or randomness in a system and is expressed in thermodynamic terms as the inability of thermal energy to be converted into mechanical work. In this work, we use different types of entropies such as Barrow entropy (BE),

Sharma-Mittal entropy (SME), and generalized construction of these entropies. We use the above-mentioned entropies to discuss the issue of baryogenesis and then we find constraints on the entropies parameters to get the physical results of $\frac{n_B}{s}$ compared to the standard observational value. To derive the modified Friedmann field equations (FFEs), we use entropies and the first law of thermodynamics. Thus, even in the presence of the typical interaction between the Ricci scalar and baryon current, this results in non-trivial modifications to the mass density and pressure content of the Universe, which provides a viable mechanism allowing for baryogenesis. Finally, we show that even in the radiation-dominant era baryon asymmetry factor (BAF) is non-zero. We conclude, BE parameter $0 \leq \Delta < 1$, SME parameters R and δ with positive $\delta \geq 4.2 \times 10^{38}$ (keeping fixed $R = 1$) while at constant $\delta = 9 \times 10^{28}$ for all values of R and for the generalized entropy parameter positive $\beta \leq 2.4 \times 10^{-28}$ (fixing $\gamma = \alpha = 5$); $\alpha \leq 3.5 \times 10^{-23}$ (for $\gamma = 1.2$ and $\beta = 3$) and $\gamma \geq 1.1 \times 10^{6}$ (at $\alpha = 3 \times 10^{-20}$, $\beta = 3$), we have physically desired results on the observational ground.

Web URL: Baryogenesis inspired by some modified entropies - IOPscience

18. Saleem, R., Aslam, M. I., & Bamba, K. (2023). A study of wormhole geometries in symmetric teleparallel gravity. Physica Scripta, 98(8), 085005.

ABSTRACT:

In this manuscript, we obtained the exact solutions of asymptotically flat wormhole (WH) geometry in the mechanism of symmetric f(Q) gravity (vanishing curvature and torsion) where Lagrangian is a function of nonmetricity Q. In this scenario, we choose two different types of f(Q) gravity models (logarithmic and exponential) along with the special choice of shape function $b(r) = \frac{r}{\exp(\gamma(r-r_0))}$, and red-shift function $\phi(r) = \frac{r_0}{2r}$. Here, γ affects the radius of curvature of WH. Under this scenario, we explore the viability of the shape function and energy conditions (ECs) of the WH solutions for each model. For both models, we determine the validity regions of ECs under some parameter spaces of the model parameters. The allowed parameter spaces for logarithmic and exponential models are illustrated in tables 1 and 2, respectively. The validity region for the null EC (NEC) represents that WH geometry in chosen f(Q) gravity models is supported by ordinary matter while exotic matter elsewhere. Furthermore, we represent the WH construction by embedding diagrams and shows that the derived WH solutions are stable for the allowed range of model parameters. Finally, it is concluded that such particular modified gravity can give us a more realistic and stable WH geometry.

Web URL: https://iopscience.iop.org/article/10.1088/1402-4896/ace3ff/meta

19. Zhang, X., Muhammad Bilal, H., Hussain, M., & Zhang, Z. (2023). On Metric Dimension of Subdivided Honeycomb Network and Aztec Diamond Network. Discrete Dynamics in Nature and Society, 2023.

ABSTRACT:

Tis paper investigates the metric dimensions of the polygonal networks, particularly, the subdivided honeycomb network, Aztec diamond as well as the subdivided Aztec diamond network. A polygon is any two-dimensional shape formed by straight lines. Triangles, quadrilaterals, pentagons, and hexagons are all representations of polygons. For instance, hexagons help us in many models to construct honeycomb network, where n is the number of hexagons from a central point to the borderline of the network. A subdivided honeycomb network (SHCN(n)) is obtained by adding additional vertices on each edge of HCN(n). An Aztec diamond network (AZN(n)) of order n is a lattice comprises of unit squares with center (a, b) satisfying $|a| + |b| \leq n$. Te subdivided Aztec diamond network (SAZN(n)) is obtained by adding additional vertices to each edge of AZN(n). In this work, our main aim is to establish the results to show that the metric dimensions of SHCN(n) and AZN(n) are 2 and 3 for n 1 and $n \geq 2$, respectively. In the end, some open problems are listed with regard to metric dimensions for k-subdivisions of HCN(n) and AZN(n)

Web URL: https://www.hindawi.com/journals/ddns/2023/7120232/

20. Guan, H., Ejaz, F., Hussain, M., & Kosari, S. (2023). Fuzzy topological invariants in uniform fuzzy graphs. Journal of Intelligent & Fuzzy Systems, (Preprint), 1-10.

ABSTRACT:

In this paper, we have defined some fuzzy topological invariants for particular types of uniform fuzzy graph. Some particular useful types of uniform fuzzy graphs are Uniform Edge Fuzzy Graph, Uniform Vertex Fuzzy Graph, Uniform Vertex-Edge Fuzzy Graph and Totally Uniform Fuzzy Graph. For each particular type we have defined different kinds of degrees in a graph in accordance with the unique nature of it. In the end, we have applied all our output results to a cellular neural fuzzy graph as an example, to verify the predicting ability of topological invariants. The aim of this paper is to define more significant fuzzy topological invariants in fuzzy graphs. Our ideas will help to create a link between fuzzy graph theory and simple (crisp) graph theory.

Web URL: https://content.iospress.com/articles/journal-of-intelligent-and-fuzzy-systems/ifs223402

21. Rana, S., Saeed, M., Qayyum, M., & Smarandache, F. (2023). Generalized plithogenic whole hypersoft set, PFHSS-Matrix, operators and applications as COVID-19 data structures. Journal of Intelligent & Fuzzy Systems, (Preprint), 1-24.

ABSTRACT:

This article is a preliminary draft for initiating and commencing a new pioneer dimension of expression. To deal with higher-dimensional data or information flowing in this modern era of information technology and artificial intelligence, some innovative super algebraic structures are essential to be formulated. In this paper, we have introduced such matrices that have multiple layers and clusters of layers to portray multi-dimensional data or massively dispersed information of the plithogenic universe made up of numerous subjects their attributes, and sub-attributes. For grasping that field of parallel information, events, and realities flowing from the micro to the macro level of universes, we have constructed hypersoft and hyper-super-soft matrices in a Plithogenic Fuzzy environment. These Matrices classify the non-physical attributes by accumulating the physical subjects and further sort the physical subjects by accumulating their non-physical attributes. We presented them as Plithogenic Attributive Subjectively Whole Hyper-Super-Soft-Matrix (PASWHSS-Matrix) and Plithogenic Subjective Attributively Whole-Hyper-Super-Soft-Matrix (PSAWHSS-Matrix). Several types of views and level-layers of these matrices are described. In addition, some local aggregation operators for Plithogenic Fuzzy Hypersoft Set (PPFHS-Set) are developed. Finally, few applications of these matrices and operators are used as numerical examples of COVID-19 data structures.

Web URL: https://content.iospress.com/articles/journal-of-intelligent-and-fuzzy-systems/ifs202792

22. Yu, X., Rehman, A. U., Ashraf, S., Hussain, M., & Faizi, S. (2023). Multiperson Decision-Making Using Consistent Interval-Valued Fuzzy Information with Application in Supplier Selection. Mathematics, 11(4), 879.

ABSTRACT:

This study describes a consistency-based approach for multiperson decision-making (MPDM) in which decision-makers' suggestions are expressed as incomplete interval-valued fuzzy preference relations. The presented approach utilizes Lukasiewicz's t-norm in conjunction with additive reciprocity to obtain comprehensive interval valued fuzzy preference relations from each expert, and the transitive closure formula also produces L-consistency. We would evaluate the consistency weights of the experts using consistency analysis. Experts are allocated final priority weights by combining the consistency weights and preset weights. A collective consistency matrix is then constructed from the weighted sum of preference matrices. After computing the possibility degrees, the normalization procedure is utilized to generate complimentary matrices, and the final ranking values of alternatives are derived as well. Finally, a numerical example demonstrates the efficacy of the suggested approach following a comparison analysis.

Web URL: https://www.mdpi.com/2227-7390/11/4/879

23. Wali, M., Arshad, S., Eldin, S. M., & Siddique, I. (2023). Numerical approximation of Atangana-Baleanu Caputo derivative for space-time fractional diffusion equations. AIMS Mathematics, 8(7), 15129-15147.

ABSTRACT:

In this study, we attempt to obtain the approximate solution for the time-space fractional linear and nonlinear diffusion equations. A finite difference approach is given for the solution of both linear and nonlinear fractional order diffusion problems. The Riesz fractional derivative in space is specifically approximated using the centered difference scheme. A system of Atangana-Baleanu Caputo equations that have been converted through spatial discretization is solved using a newly developed modified Simpson's 1/3 formula. A study of the proposed scheme is done to ascertain its stability and convergence. It has been shown that for mesh size h and time steps δt the recommended method converges at a rate of O(δt 2 + h 2). Based on graphic results and numerical examples, the application of the model is also examined.

Web URL: http://www.aimspress.com/aimspress-data/math/2023/7/PDF/math-08-07-772.pdf

24. Rizvi, S. T., Seadawy, A. R., Farah, N., & Ahmed, S. (2023). Transformation and interactions among solitons in metamaterials with quadratic-cubic nonlinearity and inter-model dispersion. International Journal of Modern Physics B, 37(09), 2350087.

ABSTRACT:

In this paper, we investigate multiple soliton interactions and other solitary wave solutions (SWS) for a perturbed nonlinear Schrödinger equation (NLSE) with negative index material having quadratic-cubic nonlinearity (NLSE-QCN). Due to its high order dispersion term, this model yields sub-picosecond impulses useful in mode-locked ring lasers. Hirota bilinear method (HBM) will be used to study soliton interaction. By controlling the parameters, we will obtain S, V, parabolic and anti-parabolic, butterfly, bright and dark shaped solitons. On the other hand, we will obtain some other solitary wave solutions with the help of Sine-Gordon expansion (SGE) scheme.

Web URL: https://www.worldscientific.com/doi/abs/10.1142/S021797922350087X

25. Nadeem, M. F., Imran, M., Afzal Siddiqui, H. M., & Azeem, M. (2023). Fault tolerance designs of interconnection networks. Peer-to-peer networking and applications, 16(2), 1125-1134.

ABSTRACT:

Multiprocessor interconnection networks are mainly required to link a significant number of stable processor memory sets, every one of which is known as a processing vertex. Due to the

cost-effectiveness, the design and utilization of multiprocessor interconnection networks have drawn attention lately. An interconnection network is extensively used in a parallel multiprocessor system to connect the processors and memory modules. In multiprocessor networks, vertices represent processors, and each processor of which is subject to complete failure. Fault tolerance is a process that ensures the working of a system to its total capacity, even if one or more of its components fail. In fault-tolerant design, backup components are used in interconnection networks to automatically take the place of the failed component, guaranteeing that the system's working continues. This paper proposed the fault-tolerant design in the form of P_j^k and C_j^k graphs, where n processing components are linked, and i of these n components creating a chain of maximum size, are used to perform the task, they can tolerate the failure of components, maintaining steady operation. In particular, we present the fault-tolerant designs of pyramid, OTIS, biswapped, and mesh-derived networks.

Web URL: https://link.springer.com/article/10.1007/s12083-023-01462-4

26. Nadeem, M. F., Iqbal, H., Siddiqui, H. M. A., & Azeem, M. (2023). Intersecting longest cycles in archimedean tilings. Algorithmica, 85(8), 2348-2362.

ABSTRACT:

In 1966 Gallai asked the following question: Do all longest paths (cycles) of a connected graph contain a common vertex? After a positive answer to Gallai's question, another question has been raised, Is there any family of graphs without Gallai's property? Menke found one such family, the square lattices. Embedding methods hold the promise to transform not just the way calculations are performed, but to significantly reduce computational costs and often used in quantum mechanics and material sciences. In this paper, we prove the existence of graphs with the empty intersection of their longest cycles as subgraphs of Archimedean lattices.

Web URL: https://link.springer.com/article/10.1007/s00453-023-01104-4

27. Zubair, M., Farooq, M., Gudekli, E., & Kousar, H. R. (2023). New traversable wormhole solutions in Einstein Gauss-Bonnet gravity. Available at SSRN 4340725.

ABSTRACT:

The present manuscript explores the existence of static wormholes in 4-Dimensional Einstein Gauss-Bonnet (4D EGB) gravity. We discuss some possibilities for constructing radial-dependent shape functions via different strategies to develop some non-conventional wormhole geometries by taking anisotropic matter sources into account. In this regards, we assume a specific form of equation of state and investigate its effects on Gauss-Bonnet (GB) coupled parameter. Next, we impose a traceless condition on anisotropic fluid distribution as well as radial dependent energy density profile to explore wormhole geometries as separate cases. It is seen that the obtainedresults can be reduced into Morris-Throne wormholes for the zero value of GB coupled parameter for anisotropicfluid distribution. In addition, we scrutinize flaring out conditions and examine asymptotically flatness constraintfor the existence of wormholes. Our

analysis shows that the weak energy condition (WEC) is satisfied for a particularrange by constraining GB coupled parameter. We study the dynamics of GB coupled parameter for bothcases $\mu>0$ and $\mu<0$. It is concluded that wormhole solutions are possible for $\mu>0$ and, in some cases,$\mu<0$.

Web URL: https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4340725

28. Zubair, M., & Farooq, M. (2023). Imprints of Casimir wormhole in Einstein Gauss–Bonnet gravity with non-vanishing complexity factor. The European Physical Journal C, 83(6), 1-20.

ABSTRACT:

This article investigates Casimir wormhole solutions in Einstein Gauss–Bonnet (EGB) gravity. We are familiar that Null energy conditions (NEC) need not be satisfied for a stable wormhole due to the existence of exotic matter. As the Casimir effect acts as a negative energy source, it can be treated as a classical applicant for the exotic matter to discuss the stable dynamics of the wormhole. This work explores the Casimir effects with the Generalized Uncertainty Principle (GUP) on wormhole geometry in EGB gravity by confining our results for D=5. We have examined two GUP procedures, e.g., Kempf, Mangano, Mann (KMM) and Dentournay, Gabriel, and Spindel (DGS). We have developed shape functions for Casimir wormholes, and GUP corrected Casimir wormholes and studied their existence. In addition, we investigate the behavior of the Gauss–Bonnet (GB) Coupled parameter and minimal uncertainty (MU) parameter on the Equation of state (EOS) parameter. The active gravitational mass and embedding diagrams for all developed shape functions are analysed. Moreover, the violation of the NEC by an exotic matter, the equilibrium forces, and the complexity factor of Casimir wormholes and GUP-corrected Casimir wormholes have also been explored.

Web URL: https://link.springer.com/article/10.1140/epjc/s10052-023-11685-7

29. Thermodynamics and Perturbative Analysis of Some Newly Developed (R, Lm, T) Theories Under the Scenario of Conserved Energy-momentum Tensor Phys.2023,71, 2300018© 2023 Wiley-VCH GmbH.2300018 (1 of 19)

ABSTRACT:

The present work is devoted to explore some interesting cosmological features of a newly proposed theory of gravity namely (R, Lm, T) theory, where R and T represent the Ricci scalar and trace of energy momentum-tensor, respectively. First, a non-equilibrium thermodynamical description is considered on the apparent horizon of the Friedmann's cosmos. The Friedmann equations are demonstrated to be equivalent to the first law of thermodynamics, i.e., TAhd$\boldsymbol{\varepsilon}'$ h + TAhdi $\boldsymbol{\varepsilon}'$ h = −dÊ + WdVˆ, where di $\boldsymbol{\varepsilon}'$ h refers to entropy production term. The constraint for validity of generalized second law of thermodynamics is also formulated and checked it for some simple well-known forms of generic function (R, Lm, T). Next, the energy bounds for this

framework and constraint the free variables by finding the validity regions for NEC and WEC are developed. Furthermore, some interesting cosmological solutions namely power law, **Λ**CDM, and de Sitter models in this theory are reconstructed. The reconstructed solutions are then examined by checking the validity of GSLT and energy bounds. Lastly, the stability of all reconstructed solutions by introducing suitable perturbations in the field equations is analyzed. It is concluded that obtained solutions are stable and cosmologically viable

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/prop.202300018

30. Zubair, M., & Raza, M. A. (2023). Rotating black hole in 4D Einstein–Gauss–Bonnet massive gravity: Shadow and center of mass energy. Physics of the Dark Universe, 40, 101200.

ABSTRACT:

This work comprises the derivation of a rotating black hole metric by applying the modified Newman– Janis algorithm to a static four dimensional black hole in Einstein–Gauss–Bonnet massive gravity. We choose several parametric values to study the influence of graviton mass m and the Gauss–Bonnet parameter α on the horizon radii and photon sphere's radii of the rotating and non-rotating black holes, respectively. By considering the Hamilton–Jacobi method, we construct the geodesic equations and by using Bardeen's procedure of impact parameters, we study the effect of graviton mass on the effective potential, shadow, distortion and energy emission rate. We find that the graviton mass has a very significant effect on the shadow and related physical observables. In the vicinity of the black hole, we investigate the collision of two uncharged particles. We compute the energy of the particles in the center of mass frame for the static and rotating BH cases. Finally, the shadow diameter is compared with Sgr. A* to obtain the constraints on the black hole parameters.

Web URL: https://www.sciencedirect.com/science/article/pii/S2212686423000341

31. Zubair, M., Azmat, H., Gudekli, E., Alhowaity, A., & Hamam, H. (2023). Implications of f (R, T) gravity on the complexity factor of a physically consistent charged anisotropic stellar model. New Astronomy, 100, 101996.

ABSTRACT:

The present manuscript throws light on the existence of an electrically charged compact stellar model and explores the behavior of complexity factor, proposed by Herrera (2018), against the selected model in the background of $f(R, T)$ gravity (R is the Ricci scalar, while T is the trace of energy–momentum tensor). The set of (R,) field equations has been solved by choosing Adler Finch–Skea solution, where the presence of electromagnetic radiations have also been considered in the stellar interior. For the space–time continuity, the boundary conditions have been described by taking Reissner–Nordström solution as exterior space–time. The physical analysis has been made by choosing the radii of PSR J 1614-2230 and SAX J 1808.4-3658, which shows

that the model is physically consistent in the realm of (R, T) gravity, and we obtain more compact stellar configurations for negative values of coupling constant λ. The implications of λ on the total mass and complexity factor of the stellar model have been explored in details. The total mass has been found maximum for $\lambda = -0.4$ and minimum for $\lambda = 0.4$. The complexity factor is increased for negative values of λ as compared to the other scenarios (i.e., $\lambda \geq 0$). The comparison of anisotropy factor and complexity factor has been made, which indicates the presence of less anisotropy in pressure distribution and more inhomogeneity in energy density of the fluid configuration for negative values of λ.

Web URL: https://www.sciencedirect.com/science/article/pii/S1384107622001786

32. Abbas, G., Övgün, A., Mahmood, A., & Zubair, M. (2023). Strong Deflection Gravitational Lensing for the Photons Coupled to the Weyl Tensor in a Conformal Gravity Black Hole. Universe 2023, 9, 130.

ABSTRACT:

In the present paper, strong deflection gravitational lensing is studied in a conformal gravity black hole. With the help of geometric optics limits, we have formulated the light cone conditions for the photons coupled to the Weyl tensor in a conformal gravity black hole. It is explicitly found that strong deflection gravitational lensing depends on the coupling with the Weyl tensor, the polarization directions, and the black hole configuration parameters. We have applied the results of the strong deflection gravitational lensing to the supermassive black holes SgrA$*$ and M87$*$ and studied the possibility of encountering quantum improvement. It is not practicable to recognize similar black holes through the strong deflection gravitational lensing observables in the near future, except for the possible size of the black hole's shadow. We also notice that by directly adopting the constraint of the measured shadow of M87$*$, the quantum effect demands immense care.

Web URL: https://inspirehep.net/files/d8d1b708131b240211d7eb0d2d689ca4

DEPARTMENT OF PHARMACY

1. Mahmood, A., Khan, L., Ijaz, M., Nazir, I., Naseem, M., Tahir, M. A., ... & Asim, M. H. (2023). Enhanced intestinal permeability of cefixime by self-emulsifying drug delivery system: in-vitro and ex-vivo characterization. Molecules, 28(6), 2827.

ABSTRACT:
Background: Cefixime (CFX) belongs to a group of third-generation cephalosporin antibiotics with low water solubility and low intestinal permeability, which ultimately leads to significantly low bioavailability. Aim: This study aimed to increase solubility, improve drug release, and intestinal permeability of CFX by loading into SEDDS. Methods: Suitable excipients were selected based on drug solubility, percent transmittance, and emulsification efficiency. Pseudo-ternary phase diagram was fabricated for the identification of effective self-emulsification region. The best probably optimized formulations were further assessed for encumbered drug contents, emulsification time, cloud point measurement, robustness to dilution, mean droplet size, zeta potential, polydispersity index (PDI), and thermodynamic and chemical stability. Moreover, in vitro drug release studies and ex vivo permeation studies were carried out and apparent drug permeability P_{app} of different formulations was compared with the marketed brands of CFX. Results: Amongst the four tested SEDDS formulations, F-2 formulation exhibited the highest drug loading of 96.32%, emulsification time of 40.37 ± 3 s, mean droplet size of 19.01 ± 1.12 nm, and demonstrated improved long-term thermodynamic and chemical stability when stored at 4 °C. Release studies revealed a drug release of 97.32 ± 4.82% within 60 min in simulated gastric fluid. Similarly, 97.12 ± 5.02% release of CFX was observed in simulated intestinal fluid within 120 min; however, 85.13 ± 3.23% release of CFX was observed from the marketed product. Ex vivo permeation studies displayed a 2.7-fold increase apparent permeability compared to the marketed product in 5 h. Conclusion: Owing to the significantly improved drug solubility, in vitro release and better antibacterial activity, it can be assumed that CFX-loaded SEDDS might lead to an increased bioavailability and antibacterial activity, possibly leading to improved therapeutic effectiveness.

Web URL: https://www.mdpi.com/1420-3049/28/6/2827

2. Asad, M., Rasul, A., Abbas, G., Shah, M. A., & Nazir, I. (2023). Self-emulsifying drug delivery systems: A versatile approach to enhance the oral delivery of BCS class III drug via hydrophobic ion pairing. PLoS One, 18(6), e0286668.

ABSTRACT:
Biopharmaceutical classification systems (BCS) class III drugs belongs to a group of drugs with high solubility in gastrointestinal (GI) fluids and low membrane permeability result in significantly low bioavailability. Self-emulsifying drug delivery systems (SEDDS) considered a

suitable candidate to enhance the bioavailability of poorly soluble drugs by improving their membrane permeability, however, incorporating hydrophilic drugs in to these carriers remained a great challenge. The aim of this study was to develop hydrophobic ion pairs (HIPs) of a model BCS class-III drug tobramycin (TOB) in order to incorporate into SEDDS and improve its bioavailability. HIPs of TOB were formulated using anionic surfactants sodium docusate (DOC) and sodium dodecanoate (DOD). The efficiency of HIPs was estimated by measuring the concentration of formed complexes in water, zeta potential determination and log P value evaluation. Solubility studies of HIPs of TOB with DOC were accomplished to screen the suitable excipients for SEDDS development. Consequently, HIPs of TOB with DOC were loaded into SEDDS and assessed the log $D_{SEDDS/release\ medium}$ and dissociation of these complexes at different intestinal pH over time. Moreover, cytotoxic potential of HIPs of TOB and HIPs loaded SEDDS formulations was evaluated. HIPs of TOB with DOC exhibited the maximum precipitation efficiency at a stoichiometric ratio of 1:5. Log P of HIPs of TOB improved up to 1500-fold compared to free TOB. Zeta potential of TOB was shifted from positive to negative during hydrophobic ion pairing (HIP). HIPs of TOB with DOC was loaded at a concentration of 1% (w/v) into SEDDS formulations. Log $D_{SEDDS/release\ medium}$ of loaded complexes in to oily droplets was above 2 and dissociated up to 20% at various pH within 4 h. Finding of this study suggested that improvement of the lipophilic character of BCS class-III drugs followed by incorporation into oily droplets can be deliberated as a promising tool to enhance the permeation across biological membranes.

Web URL: https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0286668

3. In Silico and In Vitro Studies of 4-Hydroxycoumarin-Based Heterocyclic Enamines as Potential Anti-Tumor Agents

ABSTRACT:

The present study reports the one-step synthesis of several 3-formyl-4-hydroxycouramin-derived enamines (**4a**–**4i**) in good yields (65–94%). The characterization of the synthesized compounds was carried out via advanced analytical and spectroscopic techniques, such as melting point, electron impact mass spectrometry (EI-MS), ^{1}H-NMR, ^{13}C-NMR, elemental analysis, FTIR, and UV-Visible spectroscopy. The reaction conditions were optimized, and the maximum yield was obtained at 3–4 h of reflux of the reactants, using 2-butanol as a solvent. The potato disc tumor assay was used to assess *Agrobacterium tumefaciens*-induced tumors to evaluate the anti-tumor activities of compounds (**4a**–**4i**), using Vinblastine as a standard drug. The compound **4g** showed the lowest IC_{50} value (1.12 ± 0.2), which is even better than standard Vinblastine (IC_{50} 7.5 ± 0.6). For further insight into their drug actions, an in silico docking of the compounds was also carried out against the CDK-8 protein. The binding energy values of compounds were found to agree with the experimental results. The compounds **4g** and **4h** showed the best affinities toward protein, with a binding energy value of −6.8 kcal/mol.

Web URL: https://www.mdpi.com/1420-3049/28/15/5828

4. Khalid, F. M., Ijaz, M., Mahmood, A., Waqas, M. K., Hussain, T., Asim, M. H., ... & Nazir, I. (2023). Mucoadhesive, Fluconazole-Loaded Nanogels Complexed with Sulfhydryl-β-cyclodextrin for Oral Thrush Treatment. AAPS PharmSciTech, 24(7), 194.

ABSTRACT:
The objective of this study was to generate fluconazole-loaded mucoadhesive nanogels to address the problem of hydrophobicity of fluconazole (FL). An inclusion complex was formulated with sulfhydryl-β-CD (SH-β-CD) followed by nanogels formation by a Schiff base reaction of carbopol 940 (CA-940) and gelatin (GE). For characterization, PXRD, FT-IR analysis, drug content, and phase solubility studies were performed. Similarly, nanogels were assessed for particle size, zeta potential, organoleptic, and spreadability studies. Moreover, drug contents, rheological, *in vitro* drug permeation, release kinetics, toxicity, and stability studies of nanogels were performed. Furthermore, mucoadhesive characteristics over the buccal mucosal membrane of the goat were evaluated. The nanogels formulated with a higher amount of CA-940 and subsequently loaded with the inclusion complexes of FL showed promising results. PXRD and FT-IR analysis confirmed the physical complexes by displaying a reduction in the intensity of peaks of FL. The average particle size of nanogels was in the range of 257 to 361 nm. The highest drug content of 88% was encapsulated within the FL-SH-β-CD complex. All formulations at 0.5–1% concentration displayed no toxicity to the Caco-2 cell lines. Nanogels loaded with FL-SH-β-CD complexes showed 18-fold improved mucoadhesion on the buccal mucous membrane of the goat when compared to simple nanogels. The *in vitro* permeation study exhibited significantly enhanced permeation and first-order concentration-dependent drug release was observed. On the bases of these findings, we can conclude that a mucoadhesive nanogel-based drug delivery system can be an ideal therapy for candidiasis.

Web URL: https://link.springer.com/article/10.1208/s12249-023-02653-1

5. Nousheen, K., Din, F. U., Jamshaid, H., Afza, R., Khan, S. U., Malik, M., ... & Khan, G. M. (2023). Metformin HCl-loaded transethosomal gel; development, characterization, and antidiabetic potential evaluation in the diabetes-induced rat model. Drug Delivery, 30(1), 2251720.

ABSTRACT:
Herein we designed, optimized, and characterized the Metformin Hydrochloride Transethosomes (MTF-TES) and incorporate them into Chitosan gel to develop Metformin Hydrochloride loaded Transethosomal gel (MTF-TES gel) that provides a sustained release, improved transdermal flux and improved antidiabetic response of MTF. Design Expert® software (Ver. 12, Stat-Ease, USA) was applied for the statistical optimization of MTF-TES. The formulation with Mean Particle Size Distribution (MPSD) of 165.4 ± 2.3 nm, Zeta Potential (ZP) of −21.2 ± 1.9 mV, Polydispersity Index (PDI) of 0.169 ± 0.033, and MTF percent Entrapment Efficiency (%EE) of 89.76 ± 4.12 was considered to be optimized. To check the chemical incompatibility among the MTF and other formulation components, Fourier Transform Infrared (FTIR) spectroscopy was performed and demonstrated with no chemical interaction. Surface morphology, uniformity, and segregation were evaluated through Transmission Electron Microscopy (TEM). It was revealed that the nanoparticles were spherical and round in form with intact borders. The fabricated MTF-TES has shown sustained release followed by a more pronounced effect in MTF-TES gel as compared to the plain MTF solution (MTFS) at a pH of 7.4. The MTF-TES has shown enhanced permeation followed by MTF-TES gel as compared to the MTFS at a pH of 7.4. In vivo antidiabetic assay was performed and results have shown improved antidiabetic potential of the MTF-TES gel, in contrast to MTF-gel. Conclusively, MTF-TES is a promising anti-diabetic

candidate for transdermal drug delivery that can provide sustained MTF release and enhanced antidiabetic effect.

Web URL: https://www.tandfonline.com/doi/full/10.1080/10717544.2023.2251720

6. Ramzan, M., Yousaf, A. M., & Khan, I. U. (2023). Fabrication and in vitro characterization of delafloxacin-laden electrosprayed hydroxypropyl cellulose nanoparticulated solid dispersions for enhanced aqueous solubility and release rate of the drug. *International Journal of Polymeric Materials and Polymeric Biomaterials*, 1-7.

ABSTRACT:
With the aim of fabricating and characterizing an optimized drug delivery system (DDS) for an effective administration of poorly water-soluble delafloxacin (DFX) via the oral route, several formulations of delafloxacin-laden solid dispersions (SD) were prepared employing the solvent-evaporation and electrospraying techniques concomitantly. Solubility and release rate of the drug in the SD were assessed. Solid-state characterization was performed via the X-ray diffraction (PXRD) and differential scanning calorimetric (DSC) analyses, scanning electron microscopy (SEM) and Fourier transform infrared spectroscopic (FTIR) analysis. Amongst the prepared SD, an optimized formulation consisting of DFX, HPC, and SLS at the weight ratio of (1/8/0.2) showed about 9-fold higher solubility and 13-fold faster release rate of delafloxacin as compared to delafloxacin plain drug powder (DPDP). The drug existed in the amorphous form in the spherical particles and had no covalent interaction with any of the excipients. Thus, this optimized formulation might be a useful DDS for an effective administration of DFX.

Web URL: https://www.tandfonline.com/doi/full/10.1080/00914037.2023.2289521

7. Alotaibi, B. S., Kaukab, I., Shah, S. N. H., Kharaba, Z., Naeem, A. R., Yasin, H., ... & Murtaza, G. (2024). Effect of chloroquine pre-treatment on the metoclopramide's pharmacokinetics after their co-administration. Expert Opinion on Drug Safety, (just-accepted).

ABSTRACT:

Methods

The study employed a randomized and two-phase cross-over design with 4-week washout plan. Twelve healthy male volunteers were shortlisted according to the set criteria and were administered with metoclopramide 10 mg PO and chloroquine (a total of 1500 mg) at different intervals which were (500 mg at 0, 6, and 24 h). The concentration of chloroquine and metoclopramide in the blood samples was estimated using a validated HPLC-UV technique to affirm the maximum concentration (C_{max}), time to reach C_{max} (T_{max}), and area under the curve (AUC).

Results

C_{max}, $T_{1/2}$, and AUC of metoclopramide were increased up to 20, 10, and 47.8%, respectively, by the concomitantly administering Chloroquine. Chloroquine-treated phase showed increased values of Cmax (ng/ml), AUC (ng.h/ml), and $T_{½}$ (h), i.e. 41.35 ± 1.61, 504.12 ± 66.25, and

5.72 ± 2.63, as compared to that reference phase i.e. 34.52 ± 4.92, 341.14 ± 112.8, and 5.19 ± 1.14, respectively.

Conclusions

Chloroquine was found to attenuate CYP2D6 activity in healthy Pakistani male volunteers. Hence, patients that are prescribed with metoclopramide or other CYP2D6-substrate drugs require a dose adjustment when administered with chloroquine.

Web URL: https://www.tandfonline.com/doi/abs/10.1080/14740338.2024.2387312

8. Alotaibi, B. S., Khan, M. A., Ullah, K., Yasin, H., Mannan, A., Khan, S. A., & Murtaza, G. (2024). Formulation and characterization of glipizide solid dosage form with enhanced solubility. Plos one, 19(2), e0297467.

ABSTRACT:
Glipizide, a poor water-soluble drug belongs to BCS class II. The proposed work aimed to enhance the solubility of glipizide by preparing solid dispersions, using polyvinyl pyrrolidone (PVP) and polyethylene glycol (PEG). Solvent evaporation method was used for the preparation of glipizide solid dispersions. Solid dispersions were prepared in four different drug-to-polymer ratios i.e. 1:1, 1:2, 1:3 and 1:4. Mainly effect of three polymers (PVP K30, PVP K90 and PEG 6000) was evaluated on the solubility and dissolution of glipizide. The *in-vitro* dissolution of all prepared formulations was performed under pH 6.8 at 37°C using USP type II apparatus. *In-vitro* dissolution results revealed that the formulations having high concentrations of the polymer showed enhanced solubility. Enhancements in the solubility and rate of dissolution of the drug were noted in solid dispersion formulations compared to the physical blends and pure drug. Solid dispersions containing polyvinyl pyrrolidone exhibited a more favorable pattern of drug release compared to the corresponding solid dispersions with PEG. An increase in the maximum solubility of the drug within the solid dispersion systems was observed in all instances. Two solid dispersion formulations were optimized and formulated into immediate-release tablets, which passed all the pharmacopoeial and non-pharmacopoeial tests. Fourier transformed Infrared (FTIR) spectroscopy X-ray diffraction (XRD) and Differential scanning calorimetry (DSC) were used to indicate drug: polymer interactions in solid state. Analysis of the solid dispersion samples through characterization tests indicated the compatibility between the drug and the polymer.

Web URL: https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0297467

9. Alotaibi, B. S., Kaukab, I., Shah, S. N. H., Kharaba, Z., Naeem, A. R., Yasin, H., ... & Murtaza, G. (2024). Effect of chloroquine pre-treatment on the metoclopramide's pharmacokinetics after their co-administration. Expert Opinion on Drug Safety, (just-accepted).

Methods
The study employed a randomized and two-phase cross-over design with four weeks washout plan. Twelve healthy male volunteers were shortlisted according to the set criteria and were administered with metoclopramide 10 mg PO, and chloroquine (a total of 1500 mg) at different intervals which were (500 mg at 0, 6, and 24 h). The concentration of chloroquine and metoclopramide in the blood samples was estimated using a validated HPLC-UV technique to

affirm the maximum concentration (C_{max}), time to reach C_{max} (T_{max}), and area under the curve (AUC).

Results

C_{max}, $T_{1/2}$, and AUC of metoclopramide were increased up to 20, 10, and 47.8% respectively by the concomitantly administering Chloroquine. Chloroquine-treated phase showed increased values of Cmax (ng/ml), AUC (ng.h/ml), and $T_{½}$ (h), i.e. 41.35 ± 1.61, 504.12 ± 66.25 and 5.72 ± 2.63, as compared to that Reference phase i.e. 34.52 ± 4.92, 341.14 ± 112.8, and 5.19 ± 1.14, respectively.

Conclusions

Chloroquine was found to attenuate CYP2D6 activity in healthy Pakistani male volunteers. Hence, patients that are prescribed with metoclopramide or other CYP2D6-substrate drugs require a dose adjustment when administered with chloroquine.

Web URL: https://www.tandfonline.com/doi/abs/10.1080/14740338.2024.2387312

10. Alotaibi, B. S., Khan, M. A., Ullah, K., Yasin, H., Mannan, A., Khan, S. A., & Murtaza, G. (2024). Formulation and characterization of glipizide solid dosage form with enhanced solubility. Plos one, 19(2), e0297467.

ABSTRACT:

Glipizide, a poor water-soluble drug belongs to BCS class II. The proposed work aimed to enhance the solubility of glipizide by preparing solid dispersions, using polyvinyl pyrrolidone (PVP) and polyethylene glycol (PEG). Solvent evaporation method was used for the preparation of glipizide solid dispersions. Solid dispersions were prepared in four different drug-to-polymer ratios i.e. 1:1, 1:2, 1:3 and 1:4. Mainly effect of three polymers (PVP K30, PVP K90 and PEG 6000) was evaluated on the solubility and dissolution of glipizide. The *in-vitro* dissolution of all prepared formulations was performed under pH 6.8 at 37°C using USP type II apparatus. *In-vitro* dissolution results revealed that the formulations having high concentrations of the polymer showed enhanced solubility. Enhancements in the solubility and rate of dissolution of the drug were noted in solid dispersion formulations compared to the physical blends and pure drug. Solid dispersions containing polyvinyl pyrrolidone exhibited a more favorable pattern of drug release compared to the corresponding solid dispersions with PEG. An increase in the maximum solubility of the drug within the solid dispersion systems was observed in all instances. Two solid dispersion formulations were optimized and formulated into immediate-release tablets, which passed all the pharmacopoeial and non-pharmacopoeial tests. Fourier transformed Infrared (FTIR) spectroscopy X-ray diffraction (XRD) and Differential scanning calorimetry (DSC) were used to indicate drug: polymer interactions in solid state. Analysis of the solid dispersion samples through characterization tests indicated the compatibility between the drug and the polymer.

Web URL: https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0297467

11. Alotaibi, B. S., Waqas, M. K., Saleem, S., Yasin, H., Kharaba, Z., & Murtaza, G. (2024). Rheumatoid Arthritis Treatment Potential of Stearic Acid Nanoparticles of Quercetin in Rats. ACS omega, 9(6), 7003-7011.

ABSTRACT:
This study aims to assess the anti-inflammatory potential of stearic acid nanoparticles of quercetin in an arthritic rat model. This article describes the fabrication of solid lipid nanoparticles (SLNs) using the hot melt encapsulation method, followed by the anti-inflammatory study of SLNs and other characterizations such as FTIR, XRD, and SEM. Thirty male healthy albino rats were taken and treated with FCA to induce rheumatoid arthritis. Quercetin loading of quercetin to stearic acid was confirmed by FTIR. The efficacy of quercetin-loaded SLNs to reduce inflammation was evaluated with the help of inflammatory biomarker levels. Quercetin-loaded stearic acid nanoparticles were successfully prepared by using a hot melt encapsulation method. Their average size and zeta potential were 100 nm and −25 mV, respectively. Rheumatoid arthritis was significantly ($p < 0.001$) reduced in the quercetin-loaded SLN group, as indicated by finding out the reduced levels of inflammatory mediators such as tumor necrosis factor (TNF-α) and rheumatoid factor. Quercetin-loaded stearic acid nanoparticles were found to be potentially effective in treating RA.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsomega.3c08870

12. Iqbal, Z., Xia, J., Murtaza, G., Shabbir, M., Rehman, K., Yujie, L., & Duan, L. (2023). Targeting WNT signalling pathways as new therapeutic strategies for osteoarthritis. Journal of Drug Targeting, 31(10), 1027-1049.

ABSTRACT:
Osteoarthritis (OA) is a highly prevalent chronic joint disease and the leading cause of disability. Currently, no drugs are available to control joint damage or ease the associated pain.
The *wingless-type* (*WNT*) signalling pathway is vital in OA progression. Excessive activation of the *WNT* signalling pathway is pertinent to OA progression and severity. Therefore, agonists and antagonists of the *WNT* pathway are considered potential drug candidates for OA treatment. For example, SM04690, a novel small molecule inhibitor of *WNT* signalling, has demonstrated its potential in a recent phase III clinical trial as a disease-modifying osteoarthritis drug (DMOAD). Therefore, targeting the *WNT* signalling pathway may be a distinctive approach to developing particular agents helpful in treating OA. This review aims to update the most recent progress in OA drug development by targeting the *WNT* pathway. In this, we introduce *WNT* pathways and their crosstalk with other signalling pathways in OA development and highlight the role of the *WNT* signalling pathway as a key regulator in OA development. Several articles have reviewed the Wnt pathway from different aspects. This candid review provides an introduction to *WNT* pathways and their crosstalk with other signalling pathways in OA development, highlighting the role of the *WNT* signalling pathway as a key regulator in OA development with the latest research. Particularly, we emphasise the state-of-the-art in targeting the *WNT* pathway as a promising therapeutic approach for OA and challenges in their development and the nanocarrier-based delivery of WNT modulators for treating OA.

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13. Alotaibi, B. S., Khan, A. K., Ijaz, M., Yasin, H., Nawazish, S., Sadiq, S., ... & Murtaza, G. (2023). Development, characterization, and burn wound-healing potential of neomycin-loaded clay-reinforced nanofibers. ACS omega, 8(42), 39014-39022.

ABSTRACT:

Background: Skin wounds affect millions of individuals around the world, and their treatment is expensive. **Objective**: The purpose of this study was to make neomycin-loaded CG/PVA/PAN (NCPP) nanofibers to improve wound healing. **Methods**: The NCPP nanofibers were characterized by using thermogravimetric analysis (TGA), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy, and X-ray diffraction. Drug solubility, dissolution, swelling ratio, erosion, and antibacterial studies were performed. The in vivo wound healing study of nanofibers was performed in a rabbit model and was supported by % age wound closure and histopathology. **Results**: The results of SEM showed some sort of agglomeration on the surface of fibers, while TGA showed 10% more stability for drug-loaded nanofibers. The drug permeation study indicated that the formulation with 15% PVA showed a controlled release profile of the drug. The NCPP nanofibers had an appreciable water retention capability. The NCPP nanofibers showed appreciable antibacterial activity against *Enterococcus faecalis* (Gram-positive bacteria) and *Klebsiella pneumonia* (Gram-negative bacteria). The wound healing study showed the better healing properties of NCPP nanofibers within 15 days. **Conclusion**: The findings helped us to conclude that the NCPP nanofibers were successfully fabricated and found to have a promising role in infected wound healing.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsomega.3c03593

14. Iqbal, A., Azhar, S., Murtaza, G., Bibi, R., Samreen, S., Iqbal, M. M., ... & Al-Rawi, M. B. A. (2023). Navigating Thyroid Dysfunction and Comorbidities Among University Students in Abbottabad, Pakistan–A Cross-Sectional Evaluation of Screening Tool for Thyroid Dysfunction. International Journal of General Medicine, 4193-4205.

ABSTRACT:

Background

Thyroid dysfunction has a direct role in diagnosing, and assessment and indicates the development of thyroid carcinoma. This study aimed to assess thyroid dysfunction through medical camps in different age and sex groups in students of Comsats University Abbottabad Pakistan.

Methods

In this study, a cross-sectional survey design was used. For data collection, a two-day medical camp was set in the Comsats University Abbottabad campus. The students were examined physically for symptoms of thyroid dysfunction using the survey questionnaire specifically designed for this study.

Results

The current research revealed that 78 out of 1032 students, or 7.6% of the population, had thyroid disease. Although 39.3% (=406) were found to have low risk, followed by 36.7% (n=379) had moderate risk and 23.9% (n=247) had high risk of thyroid dysfunction. Altogether, 6.1% (n=63) of the students had high blood pressure (BP), 3.2% (n=33) had high cholesterolemia, 3.4% (n=33) had angina, and 0.9% (n=9) had diabetes mellitus (DM). In relation, students who exhibit signs and symptoms that last longer than five weeks include 42.2% (n=435) who felt the need for excessive sleep, 35.3% (n=364) who felt tired, 36.8% (n=380) who had trouble concentrating and 30.1% (n=311) who had palpitations. The high risk of thyroid being seen predominantly in students between the ages of 15–20 years (31.2%, n=148), as

opposed to other age groups (p=0.001). Similar to this, women having a higher risk of thyroid disease (26.5%) than men (22.8%) (p =0.001).

Conclusion

In conclusion, few students suffer with thyroid found to have high risk of thyroid disease. This method of questionnaire-based screening for thyroid dysfunction is cost-effective, with no additive risk of adverse effects from excessive screening, and could help in the early detection of thyroid and help avoid excess costs related to thyroid dysfunction and cancer screening.

Web URL: https://www.tandfonline.com/doi/full/10.2147/IJGM.S415311

15. Asad, S., Khan, S. A., Ullah, K., Mannan, A., & Murtaza, G. (2023). Synthesis, characterization, and in-vitro evaluation of pH-responsive PEI-MAA polymeric matrices decorated with mesalazine for colonic delivery. Journal of Drug Delivery Science and Technology, 88, 104926.

ABSTRACT:

Colorectal drug delivery systems (CR-DDS) have served as efficient carriers for increasing the availability of various drugs in the colon region and are desirable to treat local diseases such as ulcerative colitis (UC), irritable bowel syndrome (IBS), and colorectal cancer (CRC). Herein we have synthesized polyethyleneimine-*co*-methacrylic acid pH-responsive hydrogels through free radical polymerization technique using ammonium persulfate as reaction initiator and mehtylenbisacrylamide as a crosslinking agent. The structure of PEI-MAA hydrogels was characterized by FT-IR, change in crystallinity was determined through X-ray diffractometry (XRD) while surface and micromorphology were determined through scanning electron microscopy (SEM). The hydrogels were subjected to a variety of tests including estimation of gelation time, sol-gel analysis, swelling experiment, drug loading and in-vitro drug release study. FTIR confirmed successful crosslinking of PEI with MAA as well as mesalazine entrapment. XRD results suggested decrease in crystallinity of drug after entrapment in the hydrogel network. Surface morphology of hydrogels illustrated a rough and uneven appearance while cross-sectional micrographs presented smooth glassy appearance with sharp edges of both unloaded and drug loaded hydrogels. The gel fraction was directly affected by an increase in the concentration of PEI (87.49%–90.35%), MAA (91.29%–92.40%) and MBA (93.77%–96.09%). The hydrogels were more responsive to alkaline pH and higher swelling indices were observed for formulations of PEI (10.28–9.23), MAA (12.79–14.42) and MBA (7.88–5.01) at pH 7.4 in comparison with acidic pH where the obtained values for polymer, monomer and crosslinker were (2.02–2.48), (3.14–2.71), (2.21–1.73) respectively. Drug entrapment was decreased with increase in concentration of PEI (72.9%–67.8%) and MBA (64%–57.4%) while MAA displayed an inverse behavior (73.2%−77.3%). while displayed an inverse effect. The drug release followed swelling pattern and there was decrease in drug release at pH 7.4 with the increase in concentration of PEI (86.03%–79.02%) and MBA (85.22%–76.42%) while MAA showed increase in drug release (87.10%–92.61%). The drug release pattern followed the Korsmeyer-Peppas model that displayed diffusion correlated with polymer chain relaxation and hydrated matrix. Based on the obtained results, PEI-MAA pH-responsive hydrogels could be a potential carrier for the colonic delivery of various hydrophilic drugs.

Web URL: https://www.sciencedirect.com/science/article/pii/S1773224723007785

16. Alotaibi, B. S., Awan, Q. T., Yasin, H., Buabeid, M., Kaleem, S., Nawazish, S., ... & Murtaza, G. (2023). Development and characterisation of MMT-reinforced polyacrylonitrile-pullulan nanofibers for controlled permeation of isotretinoin. Journal of Experimental Nanoscience, 18(1), 2221826.

ABSTRACT:
Drug nanofibers play a crucial role in ameliorating therapeutic effects, reducing toxicity, and increasing the bioavailability of drugs. This study was aimed at the fabrication of isotretinoin-loaded MMT-reinforced bi-polymeric (PAN/PU) nanofibers with varying concentrations of isotretinoin. In this study, montmorillonite (MMT)-reinforced cross-linked polyacrylonitrile and pullulan nanofibers combined with varying amounts of isotretinoin were fabricated through an electrospinning approach and investigated for their drug permeation potential. PAN-PU nanofibers were successfully integrated with the isotretinoin. The incorporation of isotretinoin into the nanofibrous structure was confirmed by FTIR and XRD. TGA study indicated the stability of the fabricated nanoparticles. The SEM results showed the beaded and smooth morphology of nanofibers. Formulation with a higher drug concentration had a non-significantly ($p > 0.05$) higher swelling ratio. Drug-loaded polymeric nanofiber erodes at a slower rate as compared to drug-free nanofibers. The *ex-vivo* permeation study of nanofibers revealed that the drug was not released all at once, but rather gradually and consistently over the period of 24 h, indicating a controlled release of the drug. In addition, the drug concentration in the nanofibers affected the permeation of the drug. According to the findings, isotretinoin-loaded MMT-reinforced bi-polymeric (PAN/PU) nanofibers with varying concentrations of isotretinoin were successfully fabricated. The fabricated nanofibers (PAN/PU) showed a promising potential for controlled permeation of drugs through rabbit skin.

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17. Pervaiz, F., Saba, A., Yasin, H., Buabeid, M., Noreen, S., Khan, A. K., & Murtaza, G. (2023). Fabrication of solid lipid nanoparticles-based patches of paroxetine and their ex-vivo permeation behaviour. Artificial Cells, Nanomedicine, and Biotechnology, 51(1), 108-119.

ABSTRACT:
Paroxetine is not suitable for oral administration due to its extensive first-pass metabolism, thus resulting in less bioavailability. This study aimed to prepare novel paroxetine-loaded solid lipid nanoparticles (SLNs) based sustained-release transdermal patches to overcome these problems by enhancing drug absorption and bioavailability. Nine formulations of paroxetine SLNs were prepared by the hot melt-homogenization method using different concentrations of glycerol monostearate (Kolliwax) and Tween 80. Then these prepared SLNs were incorporated in a matrix type transdermal patch having a matrix of ethyl cellulose and polyvinyl pyrrolidone in 3:2 with polyvinyl alcohol. The SLNs showed a particle size range of 113–230 nm and an entrapment efficiency of 85.14%. The SLNs showed sustained paroxetine release (77.86–95.63% release) up to 48 h. FTIR studies showed no interaction between drug and formulation components. Paroxetine is evenly distributed in an amorphous form in SLNs, as demonstrated by DSC as well as PXRD analysis. SLNs formulated patches showed higher drug permeation through the skin than drug-based transdermal patches., Draize patch test revealed no sign of

erythema after applying paroxetine-loaded SLN patches (score 0) as observed with the marketed product. The developed SLNs based transdermal patches showed increased permeability and sustained release behaviour.

Web URL: https://www.tandfonline.com/doi/full/10.1080/21691401.2023.2179631

18. Qaiser, R., Pervaiz, F., Shoukat, H., Yasin, H., Hanan, H., & Murtaza, G. (2023). Mucoadhesive chitosan/polyvinylpyrrolidone-co-poly (2-acrylamide-2-methylpropane sulphonic acid) based hydrogels of captopril with adjustable properties as sustained release carrier: Formulation design and toxicological evaluation. Journal of Drug Delivery Science and Technology, 81, 104291.

ABSTRACT:
Using chitosan (CS) as a mucoadhesive as well as pH-sensitive polymer, a chemically crosslinked novel CS/PVP-co-poly (AMPS) network-based hydrogels was fabricated by utilizing a radical polymerization approach followed by successful loading of captopril by applying the diffusion-aided-swelling technique. The physicochemical properties like the conformation of chemical groups, as well as physical entrapment of captopril into hydrogel network with a slight shifting of peaks illustrated by FTIR. Porous surface morphology of hydrogel aids in the uniformed entrapment of captopril molecules within matrix was demonstrated by SEM. The diminished captopril sharp peaks at 2θ = 10.91°, 17.09°, and 18.95° in the PXRD spectra of loaded hydrogel showed that drug molecules were dispersed at the molecular level and conversion of crystalline nature drug and polymer into amorphous hydrogel system which in turned aid in the dissolution profile. TGA as well as DSC illustrated the thermally stable fabricated hydrogels deterioration at a higher temperature which ensured the compact integrity of matrix. Dissolution ensured that the developed hydrogel system was inflated more and released up to 95.74% captopril at 1.2 pH. The presence of higher chitosan concentration in formulation CPAE-3 has more mucoadhesion potential (144 min) than others which confirmed that chitosan was responsible for the mucoadhesive properties. In-vivo toxicity studies proved that designed hydrogel systems were nontoxic and biocompatible. According to the results, the novel mucoadhesive, pH-sensitive, CS/PVP-co-poly (AMPS) network-based hydrogels were successfully developed for captopril to maximize the drug absorption at the stomach to achieve better bioavailability and sustained released pattern.

Web URL: https://www.sciencedirect.com/science/article/pii/S1773224723001430

19. Khan, A. K., Kaleem, S., Pervaiz, F., Sherazi, T. A., Khan, S. A., Khan, F. A., ... & Murtaza, G. (2023). Antibacterial and wound healing potential of electrospun PVA/MMT nanofibers containing root extract of Berberis lycium. Journal of Drug Delivery Science and Technology, 79, 103987.

ABSTRACT:

Background

Electrospun polymeric nanofibers have numerous attractive biomedical applications owing to their structural resemblance with the natural extracellular matrix as well as their possibility of being loaded with different bioactive agents.

Objective

The present work aimed to investigate the antibacterial activity and wound healing potential of biodegradable electrospun PVA/MMT nanofibers containing root extract of *Berberis lycium*.

Methods

The study involved the preparation and characterization of PVA/MMT nanofibers incorporated with root extract of *Berberis lycium*. The antibacterial activities of fabricated nanofiber were performed against two bacterial strains, Staphylococcus aureus and Pseudomonas aeruginosa, by agar diffusion method. The extract loaded and unloaded nanofibers were subjected to the *in vivo* wound healing studies using rabbits and compared with standard and control groups.

Results

The antibacterial potential of electrospun nanofibers was greatly influenced by the concentration of root extract, i.e. a direct relation between the antibacterial activity and extract concentration. The highest percentage of wound closure was shown by the test group as compared with the control group, showing the good healing potential of extract-loaded nanofibers.

Conclusion

The PVA/MMT nanofibers incorporated with root extract of *Berberis lycium* possess promising antibacterial activity and healing potential against burn wounds.

Web URL: https://www.sciencedirect.com/science/article/pii/S177322472200898X

20. Gul, R., Bashir, H., Sarfraz, M., Shaikh, A. J., Jardan, Y. A. B., Hussain, Z., ... & Amirzada, M. I. (2024). Human plasma derived exosomes: Impact of active and passive drug loading approaches on drug delivery. Saudi Pharmaceutical Journal, 32(6), 102096.

ABSTRACT:
The aim of the current study was to explore the potential of human plasma-derived exosomes as versatile carriers for drug delivery by employing various active and passive loading methods. Exosomes were isolated from human plasma using differential centrifugation and ultrafiltration method. Drug loading was achieved by employing sonication and freeze thaw methods, facilitating effective drug encapsulation within exosomes for delivery. Each approach was examined for its effectiveness, loading efficiency and ability to preserve membrane stability. Methotrexate (MTX), a weak acid model drug was loaded at a concentration of 2.2 µM to exosomes underwent characterization using various techniques such as particle size analysis, transmission electron microscopy and drug loading capacity. Human plasma derived exosomes

showed a mean size of 162.15 ± 28.21 nm and zeta potential of −30.6 ± 0.71 mV. These exosomes were successfully loaded with MTX demonstrated a better drug encapsulation of 64.538 ± 1.54 % by freeze thaw method in comparison 55.515 ± 1.907 % by sonication. *In-vitro* drug release displayed 60 % loaded drug released within 72 h by freeze thaw method that was significantly different from that by sonication method i.e., 99 % within 72 h (p value 0.0045). Moreover, cell viability of exosomes loaded by freeze thaw method was significantly higher than that by sonication method (p value 0.0091) suggested that there was membrane disruption by sonication method. In conclusion, this study offers valuable insights into the potential of human plasma-derived exosomes loaded by freeze thaw method suggest as a promising carrier for improved drug loading and maintenance of exosomal membrane integrity.

Web URL: https://www.sciencedirect.com/science/article/pii/S1319016424001464

21. Shah, H. S., Zaib, S., Usman, F., Sarfraz, M., Faiz, R., Rehman, S. A., ... & Nazir, I. (2024). Synthesis, characterization, pharmacological and computational evaluation of hyaluronic acid modified chebulinic acid encapsulated chitosan nanocomposite for cancer therapy. International Journal of Biological Macromolecules, 263, 130160.

ABSTRACT:

The purpose of this study was to produce hyaluronic acid customized nanoparticles with chitosan for the delivery of chebulinic acid (CLA) to enhance its anticancer potential against breast cancer. A significant portion of CLA was encapsulated (89.72 ± 4.38 %) and loaded (43.15 ± 5.61 %) within hybrid nanoparticles. The colloidal hybrid nanoparticles demonstrated a polydispersity index (PDI) of about 0.379 ± 0.112, with zeta capacitance of 32.69 ± 5.12 (mV), and an average size of 115 ± 8 (nm). It was found that CLA-CT-HA-NPs had stronger anticancer effects on MCF-7 cells (IC_{50} = 8.18 ± 3.02 μM) than pure CLA (IC_{50} = 17.15 ± 5.11 μM). The initial cytotoxicity findings were supported by additional investigations based on comet assay and flow cytometry analysis. Tumor remission and survival were evaluated in five separate groups of mice. When juxtaposed with pure CLA (3.17 ± 0.419 %), CLA-CT-HA-NPs improved survival rates and reduced tumor burden by 3.76 ± 0.811(%). Furthermore, in-silico molecular docking investigations revealed that various biodegradable polymers had several levels of compatibility with CLA. The outcomes of this study might potentially served as an effective strategy for delivering drugs in the context of breast cancer therapy.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813024009632

22. Ashfaq, M. H., Imran, M., Haider, A., Shahzadi, A., Mustajab, M., Ul-Hamid, A., ... & Ikram, M. (2023). Antimicrobial potential and rhodamine B dye degradation using graphitic carbon nitride and polyvinylpyrrolidone doped bismuth tungstate supported with in silico molecular docking studies. Scientific Reports, 13(1), 17847.

ABSTRACT:

The environmental-friendly hydrothermal method has been carried out to synthesize Bi_2WO_6 and g-C_3N_4/PVP doped Bi_2WO_6 nanorods (NRs) by incorporating different concentrations of graphitic carbon nitride (g-C_3N_4) as well as a specified quantity of polyvinylpyrrolidone (PVP). Bi_2WO_6 doped with g-C_3N_4 provides structural and chemical stability, reduces charge carriers,

degrades dyes, and, owing to lower bandgap energy, is effective for antibacterial, catalytic activity, and molecular docking analysis. The purpose of this research is the treatment of polluted water and to investigate the bactericidal behavior of a ternary system. The catalytic degradation was performed to remove the harmful rhodamine B (RhB) dye using $NaBH_4$ in conjunction with prepared NRs. The specimen compound demonstrated antibacterial activity against Escherichia coli (E. coli) at both high and low concentrations. Higher doped specimens of g-C_3N_4/PVP-doped Bi_2WO_6 exhibited a significant improvement in efficient bactericidal potential against *E. coli* (4.55 mm inhibition zone). In silico experiments were carried out on enoyl-[acylcarrier-protein] reductase (FabI) and β-lactamase enzyme for *E. coli* to assess the potential of Bi_2WO_6, PVP doped Bi_2WO_6, and g-C_3N_4/PVP-doped Bi_2WO_6 NRs as their inhibitors and to justify their possible mechanism of action.

Web URL: https://www.nature.com/articles/s41598-023-44799-9

23. Ayub, A., Ikram, M., Haider, A., Shahzadi, I., Ul-Hamid, A., Shahzadi, A., ... & Imran, M. (2023). Enhanced Industrial Dye Degradation and Antibacterial Activity Supported by the Molecular Docking Study of Yttrium and Carbon Sphere-Doped Lanthanum Oxide Nanostructures. ACS omega, 8(40), 37564-37572.

ABSTRACT:

As the population grows, the scientific community remains focused on researching new materials, methods, and devices to ensure the availability of safe drinking water. The main aim of this research was to decrease the recombination rate of the charge carriers of La_2O_3 and enhance the catalytic and antimicrobial activity by employing Y/Cs- doped La_2O_3, respectively. In the current study, different concentrations of yttrium (Y) and a fixed amount of carbon spheres (Cs) doped into lanthanum oxide (La_2O_3) nanostructures (NSs) were synthesized by the coprecipitation technique. Cs are used as a cocatalyst as they have a high surface area and small size attributed to increased active sites and decreased recombination rate. Moreover, Y was further incorporated as it activates the generation of reactive oxygen species in the inhibition zone, enhancing the antibacterial activity and reducing the emission intensity. Advanced techniques were utilized to determine the structural properties, optical emission and absorption, elemental composition, and *d*-spacing of the synthesized samples. The reported ternary catalyst works efficiently, improving the catalytic activity and bactericidal potential. Moreover, in silico molecular docking studies, Cs-doped La_2O_3 and Y/Cs-doped La_2O_3 nanostructures toward DNA gyrase *Escherichia coli* showed good efficacy for antibacterial activity.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsomega.3c05938

24. Khan, L., Ikram, M., Haider, A., Shahzadi, A., Ul-Hamid, A., Ullah, H., ... & Shahzadi, I. (2023). Carbon spheres/polyvinylpyrrolidone doped MnO2 nanorods served as dye degrader and antibacterial activity with evidential molecular docking. Surfaces and Interfaces, 42, 103372.

ABSTRACT:

The present study synthesized carbon sphere (CS) and polyvinylpyrrolidone (PVP) doped MnO_2 nanorods via co-precipitation technique. Using a systematic approach, this research

investigates the deliberate doping of carbon spheres at 2 and 4 wt.% concentrations into a predetermined quantity of PVP-doped MnO_2 nanorods (NRs). The motive of this work was to reduce the recombination rate and inhibit the dimension of NRs that caused to increase in the catalytic reduction of methylene blue and microbicidal action of MnO_2 NRs confirmed by molecular docking analysis. Several characterization techniques were utilized to check the effect of doping agents (CS and PVP) on the structural, morphological and optical characteristics of MnO_2. The XRD pattern evidenced that MnO_2 had an orthorhombic framework, and incorporating PVP and CS reduced the crystallinity of NRs. The electronic spectra revealed the blue shift, assigned to increase band gap energy by the addition PVP and CS. TEM analysis confirmed the formation of a network of MnO_2 nanorods and decreased size with the integration of dopants. CS and PVP-doped MnO_2 NRs significantly improved their microbicidal effectiveness towards *Escherichia coli* (*E. coli*) measured in an inhibitory zone mm and catalytic performance. The enigma behind these bactericidal effects was recently unraveled by in silico assertions regarding these doped NRs for targeted enzymes (i.e., DNA gyrase and β-lactamase).

Web URL: https://www.sciencedirect.com/science/article/pii/S2468023023007423

25. Shahzadi, I., Islam, M., Saeed, H., Haider, A., Shahzadi, A., Rathore, H. A., ... & Ikram, M. (2023). Synthesis of curcuma longa doped cellulose grafted hydrogel for catalysis, bactericidial and insilico molecular docking analysis. International Journal of Biological Macromolecules, 253, 126827.

ABSTRACT:
Curcumin (diferuloylmethane), the primary curcuminoid in turmeric rhizome, has been acknowledged as a bioactive compound for numerous pharmacological activities. Nonetheless, the hydrophobic nature, rapid metabolism, and physicochemical and biological instability of this phenolic compound correspond to its poor bioavailability. So, recent scientific advances have found many components and strategies for enhancing the bioavailability of curcumin with the inclusion of biotechnology and nanotechnology to address its existing limitations. Therefore, In this study, copolymerized aqua-gel was synthesized by graft polymerization of poly-acrylic acid (P-AA) on cellulose nanocrystals (CNC), after that *Curcuma longa* (Cur) was incorporated as dopant (5, 10, 15, and 25 mg) in hydrogel (Cur/C-P) as a stabilizing agent for evaluation of bacterial potential and sewage treatment. The antioxidant tendency of 25 mg Cur/C-P was much higher (72.21 %) than other samples and displayed a catalytic activity of up to 93.89 % in acidic conditions and optimized bactericidal inclinations toward gram-positive bacterial strains. Furthermore, ligand binding was conducted against targeted protein enoyl-[acylcarrier-protein] reductase (FabI) enzyme to comprehend the putative mechanism of microbicidal action of CNC-PAA (Csingle bondP), Cur/C-P, and curcumin. Our outcomes suggest that 25 mg Cur/C-P hydrogels are plausible sources for hybrid, multifunctional biological activity.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813023037248

26. Rani, S., Imran, M., Haider, A., Shahzadi, A., Ul-Hamid, A., Somaily, H. H., ... & Ikram, M. (2023). Dye Degradation, Antimicrobial Activity, and Molecular Docking Analysis of Samarium-Grafted Carbon Nitride Doped-Bismuth Oxobromide Quantum Dots. Global Challenges, 7(12), 2300118.

ABSTRACT:
Various concentrations of samarium-grafted-carbon nitride (Sm-g-C_3N_4) doped-bismuth oxobromide (BiOBr) quantum dots (QDs) are prepared by the co-precipitation method. Elemental evaluation, morphological, optical, and functional group assessment are studied employing characterization techniques. Based on the XRD pattern analysis, it is determined that BiOBr exhibits a tetragonal crystal structure. The electronic spectroscopy revealed an absorption peak for BiOBr at 315 nm and the bandgap energy (E_g) decreasing from 3.9 to 3.8 eV with the insertion of Sm-g-C_3N_4. The presence of vibrational modes related to BiOBr at 550 cm^{-1} is confirmed through FTIR spectra. TEM revealed that pure BiOBr possessed non-uniform QDS, and agglomeration increased with the addition of Sm-g-C_3N_4. The catalytic performance of Sm-g-C_3N_4 into BiOBr (6 mL) in a neutral medium toward rhodamine B exhibited excellent results (99.66%). The bactericidal activity is evaluated against multi-drug resistance (MDR) *Escherichia coli* once the surface area is increased by dopant and the measured inhibition zone is assessed to be 3.65 mm. Molecular docking results supported the in vitro bactericidal potential of Sm-g-C_3N_4 and Sm-g-C_3N_4 doped-BiOBr as DNA gyrase$_{E.\ coli}$ inhibitors. This study shows that the novel Sm-g-C_3N_4 doped-BiOBr is a better catalyst that increases specific semiconductor's catalytic activity (CA).

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/gch2.202300118

27. Arshad, S., Imran, M., Haider, A., Shahzadi, A., Saeed, H., Ul-Hamid, A., ... & Ikram, M. (2024). Evaluation of Bactericidal Potential and Catalytic Dye Degradation of Yttrium/Graphitic Carbon Nitride Doped Nickel Oxide Nanostructures. Journal of Inorganic and Organometallic Polymers and Materials, 34(5), 2017-2029.

ABSTRACT:
In this research work, nickel dioxide (NiO_2) with a fixed quantity of graphitic carbon nitride (g-C_3N_4) and various concentrations of yttrium (Y) (2, 4 wt%) were synthesized via the coprecipitation method. The main objective is to degrade hazardous dyes such as Rhodamine B (RhB) with synthetic material and to assess antibacterial and catalytic activity with molecular docking analysis of the synthesized Y/g-C_3N_4-doped NiO_2 nanostructures (NSs). A series of characterizations for optical, morphological, structural, and compositional analysis of prepared NSs were monitored to better understand the obtained samples. X-ray diffraction pattern evaluated the hexagonal structure of NiO_2. Fourier transform infrared spectra demonstrated the prescence of bending and stretching vibration modes. Upon the incorporation of Y and g-C_3N_4, no visible transmittance shift was observed. The high resolution transmission electron microscopy micrographs affirmed the formation of agglomerated NiO_2 NSs with few rod-like shapes, also assured by EDS elemental configuration. The UV–vis spectra revealed a redshift upon including Y and g-C_3N_4 into NiO_2, leading the band gap energy to decrease from 3.6 to 3.4 eV. The catalytic efficacy of prepared samples was examined against Rhodamine B (RhB) dye in the prescence of reducing agent. In an acidic medium, the highest catalytic degradation rate of 99.85% was achieved by 4% Y/g-C_3N_4–NiO_2, ascribed to increased production of H^+ ions absorbed over the NSs surface. Moreover, the antimicrobial efficacy of synthesized NSs was evaluated against *Escherichia coli* (*E.coli*) bacteria and was observed as 3.15 mm. In silico

docking studies of g-C_3N_4/NiO_2 and Y/g-C_3N_4–NiO_2 NSs for dihydrofolatereductase (DHFR) and dihydropteroate synthase (DHPS) of *E.coli* postulated inhibition of the enzymes above as a possible mechanism in addition to their microbicidal activity.

Web URL: https://link.springer.com/article/10.1007/s10904-023-02944-x

28. Faisal, M. Z. U. R., Imran, M., Haider, A., Shahzadi, A., Baz, S., Ul-Hamid, A., ... & Ikram, M. (2024). Catalytic degradation of rhodamine blue and bactericidal action of AgBr and chitosan-doped CuFe2O4 nanostrucutres evidential molecular docking analysis. International Journal of Biological Macromolecules, 258, 128885.

ABSTRACT:
The harmful cationic dyes present in industrial waste significantly decrease the effectiveness of remedy operations. Considering the horrendous impact of these dyes on the environment and biodiversity, silver bromide (AgBr) and chitosan (CS) doped copper ferrite ($CuFe_2O_4$) nanostructures (NSs) were prepared by the co-precipitation route. In this work, The surface characteristics of $CuFe_2O_4$ can be altered by CS, potentially enhancing its catalytic reaction compatibility. The functional groups in CS interact with the surface of $CuFe_2O_4$, influencing its catalytic behavior. AgBr can have an impact on the dynamics of charge carriers in the composite. Better charge separation and transfer which is essential for catalytic processes. The catalytic degradation of RhB was significantly enhanced (100 %) using 4 wt% of AgBr-doped CS-$CuFe_2O_4$ catalysts in a basic medium. The significant inhibitory zones (9.25 to 17.95 mm) inhibitory in maximum doses were seen against Gram-positive bacteria (*S. aureus*). The bactericidal action of AgBr/CS-doped $CuFe_2O_4$ NSs against DNA $gyrase_{S.aureus}$ and tyrosyl-tRNAsynthetase *S. aureus* was rationalized using molecular docking studies, which supported their function as inhibitor

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813023057847

29. Ikram, M., Haider, A., Shahzadi, A., Mustajab, M., Fayyaz, M., Ul-Hamid, A., ... & Ahmed, B. A. (2024). Efficient scalable co-precipitated carbon dots and silver bromide doped manganese dioxide for catalytic and antimicrobial activity with evidential in-silico analysis. Surfaces and Interfaces, 44, 103677.

ABSTRACT:
In this research, a co-precipitation approach was used to synthesize manganese oxide (MnO_2) nanorods (NRs) doped with varying concentrations (2, 4 wt.%) of silver bromide (AgBr) and fixed amounts of carbon dots (CDs). CDs exhibit high photostability and a high electron transfer rate. AgBr can improve the activity of metal oxide owing to its electron-trapping effect. The new characteristics of as-prepared AgBr/CDs doped MnO_2 NRs have a larger surface area, charge transport capabilities, and lower recombination chances, associating the synthesized material as a suitable choice for environmental cleanup. The removal of organic dye pollutants from wastewater and the elimination of harmful bacteria by the use of antibacterial activity were the goals of this research. The NRs demonstrated outstanding catalytic activity (CA) against rhodamine B (RhB) dye degradation. AgBr/CDs-doped MnO_2 nanocatalyst indicates efficient dye degradation (96.39 %) in an acidic medium relative to other basic and neutral media. The fundamental components for generating

reactive oxygen species (ROS) are electrons and hole pairs responsible for killing pathogenic bacteria. Compared to ciprofloxacin the substantial inhibition zones against *Escherichia coli (E. coli)* bacteria were measured at 2.95 mm. In silico molecular docking study of AgBr/CDs-doped MnO_2 NRs proposed as promising DNA gyrase *E. coli* inhibitors.

Web URL: https://www.sciencedirect.com/science/article/pii/S246802302301043X

30. Hussain, S., Ikram, M., Haider, A., Shahzadi, A., Parveen, S., Shahzadi, I., ... & Nabgan, W. (2024). Dye degradation and antibacterial performance of carbon sphere and silver doped-LZH; in silico molecular docking evaluation. Journal of Photochemistry and Photobiology A: Chemistry, 447, 115242.

ABSTRACT:
In the present work, a fixed quantity of carbon sphere (CS) with 2 and 4 wt% of silver (Ag) was effectively integrated into layered zinc hydroxide (LZH) using co-precipitation method. This study aimed to check rhodamine dye degradation using catalysis and evaluate the antibacterial activity of LZH and Ag/CS-LZH with molecular docking analysis. To improve catalytic efficiency, CS and Ag were doped into LZH. Various characterizations of LZH and Ag/CS-LZH were assessed to determine the optical, structural, and morphological features. (4. wt%) Ag/CS-LZH demonstrated high catalytic activity (calculated as 87.28%) in an acidic medium with a significant inhibition zone against *Escherichia coli (E. coli)*. The antimicrobial activity of CS-LZH and Ag/CS-LZH nanostructures against $DHFR_{E.\ coli}$ and $DHPS_{E.\ coli}$ was explicated by molecular docking investigations.

Web URL: https://www.sciencedirect.com/science/article/pii/S1010603023007074

31. Shaheen, F., Imran, M., Haider, A., Shahzadi, A., Moeen, S., Ul-Hamid, A., ... & Ikram, M. (2024). Size-controlled synthesis of La and chitosan doped cobalt selenide nanostructures for catalytic and antibacterial activity with molecular docking analysis. International Journal of Biological Macromolecules, 263, 130096.

ABSTRACT:
Co-precipitation method was adopted to synthesize ternary heterostructure catalysts La/CS-CoSe NSs (lanthanum/chitosan-cobalt selenide nanostructures) without the use of a surfactant. During synthesis, a fixed amount (3 wt%) of CS was doped with 2 and 4 wt% La to control the growth, recombination rate and stability of CoSe NSs. The doped samples served to enhance the surface area, porosity and active sites for catalytic degradation of rhodamine B dye and antibacterial potential against *Staphylococcus aureus* (*S. aureus*). Additionally, the synthesized catalysts were examined for morphological, structural and optical characteristics to assess the influence of dopants to CoSe. XRD spectra verified the hexagonal and cubic structure of CoSe, whereas the porosity of the undoped sample (CoSe) increased from 45 to 60 % upon incorporation of dopants (La and Cs). Among the samples analyzed during this study, 4 % La/CS-CoSe exhibited significant bactericidal behavior as well as the highest catalytic reduction of rhodamine B dye in a neutral environment. Molecular docking analysis was employed to elucidate the underlying

mechanism behind the bactericidal activity exhibited by CS-CoSe and La/CS-CoSe NSs against $DHFR_{S.\ aureus}$ and DNA $gyrase_{S.\ aureus}$.

Web URL: https://www.sciencedirect.com/science/article/pii/S0141813024008997

32. Siddique, M. A. B., Imran, M., Haider, A., Shahzadi, A., Ul-Hamid, A., Nabgan, W., ... & Mahmood, A. (2024). Enhancing catalytic and antibacterial activity with size-controlled yttrium and graphene quantum dots doped MgO nanostructures: A molecular docking analysis. Materials Today Sustainability, 25, 100690.

ABSTRACT:
Designing efficient catalysts that possess large number of active sites, high catalytic activity and selectivity while also exhibiting strong antimicrobial activity is a challenging task because of poor control over material fabrication. Therefore, developing new and innovative approaches for the synthesis of catalytic materials is crucial for addressing these challenges. Here, we report the controlled fabrication of GQDs/Y-doped MgO nanoparticles achieved by co doping of yttrium (Y) and graphene quantum dots (GQDs) in magnesium oxide (MgO) based nanostructures (NSs) using the co-precipitation method. The co-doping of GQDs and Y was controlled by manipulating the ratio of precursors where introduction of GQD resulted in higher surface area and enhanced conductivity while the doping of Y enhanced the number of active sites in the final product. The GQDs/Y-doped MgO exhibited an average particle size of ~50 nm and a bandgap of 3.6 eV. Owing to these excellent characteristics, the GQDs/Y-doped MgO was utilized as a catalyst for treatment of the organic pollutants from water as well as antibacterial activity. The modified GQDs/Y-doped MgO nanostructure exhibited excellent activity of over 99.9 % for dye removal and versatility in a broad range of pH which clearly indicated the application in a range of different environments. Furthermore, the GQDs/Y-doped MgO exhibited excellent antibacterial activity against *Escherichia Coli* (*E. Coli*) bacteria. To gain further insights into the origins of this excellent activity response, the molecular docking simulations (MDS) is utilized against DNA gyrase and FabI (two enzymes critical to nucleic acid and fatty acid biosynthesis, respectively), to uncover the mechanism behind the observed antibacterial effects. In summary, the modified catalyst provides a pathway to design highly efficient catalysts for all pH range water treatment as well as good activity against microbes.

Web URL: https://www.sciencedirect.com/science/article/pii/S2589234724000265

33. Haq, E. U., Imran, M., Haider, A., Shahzadi, A., Habib, A., Ul-Hamid, A., ... & Ikram, M. (2024). Catalytic action and bactericidal behavior of samarium/carbon spheres-doped manganese oxide nanostructures and their molecular docking analysis. Journal of Alloys and Compounds, 973, 172760.

ABSTRACT:
The co-precipitation technique was adapted to synthesize different concentrations (2 % and 4 %) of samarium (Sm) doped constant equates of carbon spheres (Cs) and manganese oxide (MnO_2). The principal objective of this investigation is to demonstrate confirmation that Sm/Cs-doped MnO_2 nanostructures (NSs) owned antibacterial and catalytic attributes. Reduction in surface area manifested to agglomeration, NSs faces become inaccessible to initiate a reaction, can be

overcome upon doping of Sm. Sm has the potential to increase the activity of metal oxide ascribed to its electron trapping effect. The structural morphologies, optical properties, functional groups, elemental composition, and d-spacing were determined by applying various characterizations. With the incorporation of CS and Sm, UV–vis spectra shifted towards lower wavelength and band gap energy (Eg) was reduced. MnO_2 possessed orthorhombic structure, according to the XRD pattern and TEM exhibited long Burr-like morphology of undoped MnO_2. SAED image illustrated that MnO_2 is polycrystalline. 4 % Sm/CS doped MnO_2 revealed the highest degradation (91 %) in a neutral environment. Furthermore, 4 % Sm/Cs doped-MnO_2 revealed an inhibitory zone of 2.85 mm against *Escherichia coli* (*E. coli*). Additionally, an analysis of molecular docking revealed a binding interface with NRs and the functional domains of certain cellular proteins. Results indicated that Cs-doped MnO_2 and Cs/Sm-doped MnO_2 NRs are the most potent DNA gyrase and FabB enzyme inhibitors.

Web URL: https://www.sciencedirect.com/science/article/pii/S092583882304063X

34. Manzoor, M., Solangi, M., Perveen, S., Salar, U., Naz, F., Iqbal, J., ... & Khan, K. M. (2024). Exploring tricycle acridines as prospective urease inhibitors: synthesis via microwave assistance, in vitro evaluation, kinetic profiling, and molecular docking investigations. Journal of the Iranian Chemical Society, 21(4), 1163-1183.

ABSTRACT:

The current research deals with the microwave-assisted green synthesis of two acridine-based libraries and in vitro urease inhibitory activities. The first library is based on 9-phenyl acridine **1**–**13** derivatives, while the second is based on 10*H*-acridin-9-one **14**–**33** derivatives. All compounds were characterized using FTIR, EI-MS, ^{1}H-NMR, and CHNX techniques. As a result of in vitro evaluation of the synthesized derivatives, most compounds showed potent inhibitory activity against urease with IC_{50} values ranging from 0.91 to 11.84 µM. Thiourea was used as the standard ($IC_{50} = 19.43 \pm 0.18$ µM). The structure–activity relationship (SAR) was established to identify key relationships between studied compounds' chemical structure and biological activity. The kinetic studies revealed a competitive mode of inhibition by the compounds. In addition, molecular docking and MD simulation studies were conducted to determine the different interactions between the ligands (compounds) and the enzyme's active site for the retention time of the ligand into the active pocket of the protein. Thus, it is well-known that inhibiting the urease enzyme activity effectively treats infections caused by *Helicobacter pylori*. This study has identified that these synthetic acridines may serve as promising lead candidates as urease inhibitors.

Web URL: https://link.springer.com/article/10.1007/s13738-024-02990-3

35. Seraj, F., Khan, K. M., Iqbal, J., Imran, A., Hussain, Z., Salar, U., ... & Taha, M. (2023). Evaluation of synthetic aminoquinoline derivatives as urease inhibitors: in vitro, in silico and kinetic studies. Future Medicinal Chemistry, 15(18), 1703-1717.

ABSTRACT:

Background

Quinoline and acyl thiourea scaffolds have major chemical significance in medicinal chemistry. Quinoline-based acyl thiourea derivatives may potentially target the urease enzyme.

Materials & methods

Quinoline-based acyl thiourea derivatives **1**–**26** were synthesized and tested for urease inhibitory activity.

Results

19 derivatives (**1**–**19**) showed enhanced urease enzyme inhibitory potential (IC_{50} = 1.19–18.92 μM) compared with standard thiourea (IC_{50} = 19.53 ± 0.032 μM), whereas compounds **20**–**26** were inactive. Compounds with OCH_3, OC_2H_5, Br and CH_3 on the aryl ring showed significantly greater inhibitory potential than compounds with hydrocarbon chains of varying length. Molecular docking studies were conducted to investigate ligand interactions with the enzyme's active site.

Conclusion

The identified hits can serve as potential leads against the drug target urease in advanced studies.

Web URL: https://www.tandfonline.com/doi/abs/10.4155/fmc-2023-0168

36. Basri, R., Fatima, S., Jalil, S., Imran, A., Fatima, N., Syed, A., ... & Shafiq, Z. (2023). 2-Oxoquinoline-based-thiosemicarbazones as multitargeting neurotherapeutics against Alzheimer's disease: In vitro and in silico studies of MAO and ChE inhibitors. Archiv der Pharmazie, 356(11), 2300430.

ABSTRACT:

Alzheimer's disease (AD) presents a multifactorial neurological disorder with multiple enzyme involvement in its onset. Conventional monotherapies fall short in providing long-term relief, necessitating the exploration of alternative multitargeting approaches to address the complexity of AD. Therefore, the design, synthesis, and in vitro and in silico evaluation of 2-oxoquinoline-based thiosemicarbazones **9a–r** as multipotent analogs, able to simultaneously inhibit the cholinesterase (ChE) and monoamine oxidase (MAO) enzymes for the potential treatment of AD, are reported. In the in vitro experimental evaluation of MAO and ChE inhibition, all tested compounds demonstrated remarkable potency exhibiting nonselective inhibition of both MAO-A and MAO-B, and selective inhibition of acetylcholinesterase (AChE) over butyrylcholinesterase (BChE), with **9d**, **9j**, and **9m** evolving as lead compounds for MAO-A, MAO-B, and AChE, displaying IC_{50} values of 0.35 ± 0.92, 0.50 ± 0.02, and 0.25 ± 0.13 μM, respectively. Moreover, the kinetic studies revealed that all tested compounds inhibited all three enzymes through a competitive mode of inhibition. Furthermore, the molecular docking studies of the most active compounds revealed several crucial interactions, particularly hydrogen bonding interactions. These interactions were observed between the nitrogen and sulfur atoms of thiosemicarbazone and the nitrogen and oxygen atoms of the quinoline ring with various amino acids, suggesting the strong interactions of these compounds with the enzymes

Web URL: https://onlinelibrary.wiley.com/doi/full/10.1002/ardp.202300430

37. Mehmood, Y., Shahid, H., Barkat, K., Arshad, N., Rasul, A., Uddin, M. N., & Kazi, M. (2023). Novel Hydrolytic Degradable Crosslinked Interpenetrating Polymeric Networks

(IPNs): An Efficient Hybrid System to Manage the Controlled Release and Degradation of Misoprostol. Gels, 9(9), 697.

ABSTRACT:

Purpose

The goal of this study was to make pH-sensitive HPMC/Neocel C19-based interpenetrating polymeric networks (IPNs) that could be used to treat different diseases. An assembled novel carrier system was demonstrated in this study to achieve multiple functions such as drug protection and self-regulated release.

Methods

Misoprostol (MPT) was incorporated as a model drug in hydroxyl-propyl-methylcellulose (HPMC)- and Neocel C19-based IPNs for controlled release. HPMC- and Neocel C19-based IPNs were fabricated through an aqueous polymerization method by utilizing the polymers HPMC and Neocel C19, the initiator ammonium peroxodisulfate (APS), the crosslinker methylenebisacrylamide (MBA), and the monomer methacrylic acid (MAA). An IPN based on these materials was created using an aqueous polymerization technique. Samples of IPN were analyzed using scanning electron microscopy (SEM), atomic force microscopy (AFM), differential scanning calorimetry (DSC), thermal analysis (TGA), and powder X-ray diffraction (PXRD). The effects of the pH levels 1.2 and 7.4 on these polymeric networks were also studied in vitro and through swelling experiments. We also performed in vivo studies on rabbits using commercial tablets and hydrogels.

Results

The thermal stability measured using TGA and DSC for the revised formulation was higher than that of the individual components. Crystallinity was low and amorphousness was high in the polymeric networks, as revealed using powder X-ray diffraction (PXRD). The results from the SEM analysis demonstrated that the surface of the polymeric networks is uneven and porous. Better swelling and in vitro results were achieved at a high pH (7.4), which endorses the pH-responsive characteristics of IPN. Drug release was also increased in 7.4 pH (80% in hours). The pharmacokinetic properties of the drugs showed improvement in our work with hydrogel. The tablet MRT was 13.17 h, which was decreased in the hydrogels, and its AUC was increased from 314.41 ng h/mL to 400.50 ng h/mL in hydrogels. The blood compatibility of the IPN hydrogel was measured using different weights (100 mg, 200 mg, 400 mg, and 600 mg; 5.34%, 12.51%, 20.23%, and 29.37%, respectively).

Conclusions

As a result, IPN composed of HPMC and Neocel C19 was successfully synthesized, and it is now possible to use it for the controlled release of MPT.

Web URL: https://www.mdpi.com/2310-2861/9/9/697

38. Mehmood, Y., Shahid, H., Arshad, N., Rasul, A., Jamshaid, T., Jamshaid, M., ... & Kazi, M. (2023). Amikacin-loaded Chitosan Hydrogel Film cross-linked with folic acid for Wound Healing Application. Gels, 9(7), 551.

ABSTRACT:

Purpose

Numerous carbohydrate polymers are frequently used in wound-dressing films because they are highly effective materials for promoting successful wound healing. In this study, we

prepared amikacin (AM)-containing hydrogel films through the cross-linking of chitosan (CS) with folic acid along with methacrylic acid (MA), ammonium peroxodisulfate (APS), and methylenebisacrylamide (MBA). In the current studies, an effort has been made to look at the possibilities of these materials in developing new hydrogel film wound dressings meant for a slow release of the antibiotic AM and to enhance the potential for wound healing.

Methods

Free-radical polymerization was used to generate the hydrogel film, and different concentrations of the CS polymer were used. Measurements were taken of the film thickness, weight fluctuation, folding resistance, moisture content, and moisture uptake. HPLC, FTIR, SEM, DSC, and AFM analyses were some of the different techniques used to confirm that the films were successfully developed.

Results

The AM release profile demonstrated regulated release over a period of 24 h in simulated wound media at pH 5.5 and 7.4, with a low initial burst release. The antibacterial activity against gram-negative bacterial strains exhibited substantial effectiveness, with inhibitory zones measuring approximately 20.5 ± 0.1 mm. Additionally, in vitro cytocompatibility assessments demonstrated remarkable cell viability, surpassing 80%, specifically when evaluated against human skin fibroblast (HFF-1) cells.

Conclusions

The exciting findings of this study indicate the promising potential for further development and testing of these hydrogel films, offering effective and controlled antibiotic release to enhance the process of wound healing.

Web URL: https://www.mdpi.com/2310-2861/9/7/551

39. Alfatama, M., Shahzad, Y., & Choukaife, H. (2024). Recent advances of electrospray technique for multiparticulate preparation: Drug delivery applications. Advances in Colloid and Interface Science, 103098.

ABSTRACT:

The electrospray (ES) technique has proven to be an effective and a versatile approach for crafting drug delivery carriers with diverse dimensions, multiple layers, and varying morphologies. Achieving the desired particle properties necessitates careful optimization of various experimental parameters. This review delves into the most prevalent ES system configurations employed for this purpose, such as monoaxial, coaxial, triaxial, and multi-needle setups with solid or liquid collector. In addition, this work underscores the significance of ES in drug delivery carriers and its remarkable ability to encapsulate a wide spectrum of therapeutic agents, including drugs, nucleic acids, proteins, genes and cells. Depth examination of the critical parameters governing the ES process, including the choice of polymer, surface tension, voltage settings, needle size, flow rate, collector types, and the collector distance was conducted with highlighting on their implications on particle characteristics, encompassing morphology, size distribution, and drug encapsulation efficiency. These insights illuminate ES's adaptability in customizing drug delivery systems. To conclude, this review discusses ES process optimization strategies, advantages, limitations and future directions, providing valuable guidance for researchers and practitioners navigating the dynamic landscape of modern drug delivery systems.

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40. Javed, E., Khan, H. M., Shahzad, Q., Shahzad, Y., Yasin, H., Ul-Haq, Z., ... & Khan, A. A. (2023). Phytochemical characterization and anti-arthritic potential of Croton bonplandianus leaves extract: In-vivo and in-silico approach. Saudi Pharmaceutical Journal, 31(12), 101860.

ABSTRACT:
Croton bonplandianus, a natural source traditionally used for treating various illnesses, including rheumatoid arthritis, was evaluated in this study. The effects of ethanolic extracts (CBEE) and aqueous fractions (CBAF) of *C. bonplandianus* leaves on arthritis-induced inflammation were studied using an albino rat model of inflammation induced by Freund's complete adjuvant. Eight test groups (n = 5 per group) and one vehicle control were used to evaluate the antiarthritic effects of different doses of CBEE and CBAF (125 $mg.kg^{-1}$, 250 $mg.kg^{-1}$, and 500 $mg.kg^{-1}$) on days 5, 10, 15, and 20 compared to arthritic and vehicle controls. Arthritis severity was assessed using macroscopic arthritis grading, histological analysis, body weights, and paw thickness. CBEE and CBAF were found to reduce the prevalence of arthritis, increase body weight, and decrease paw inflammation compared to the vehicle control group by the 23rd day. In addition, they showed no effect on biochemical parameters, but a significant difference ($p < 0.05$) in hematological parameters compared to the arthritic control group. The study identified Hentriacontane compound as a potential contributor to the anti-inflammatory effect of *C. bonplandianus*, as it showed the lowest dock score for IL-1β and IL-6. Palmitoylethanol amide was identified as a potential contributor to the anti-inflammatory effect of TNF-α. Gene expression of IL-6, IL-1β, and TNF-α was down-regulated significantly ($p < 0.05$) in a dose-dependent manner in all treatment groups compared to the arthritic control group. In conclusion, this study validated the anti-arthritic and anti-inflammatory properties of CBEE and CBAF in a time and dose-dependent manner.

Web URL: https://www.sciencedirect.com/science/article/pii/S1319016423003559

41. Gerber, M., Oosthuysen, E., van Jaarsveld, J. R., Shahzad, Y., & du Plessis, J. (2023). Grapeseed oil nanoemulsions and nanoemulgels for transdermal delivery of a series of statins. Journal of Drug Delivery Science and Technology, 88, 104900.

ABSTRACT:
Cholesterol, a natural substance present in the body, is an integral part of the cell wall for its sustenance and functionality [1]. Hypercholesteremia represents elevated serum cholesterol levels, shortage of high-density lipoproteins (HDL), and abundance of low-density lipoproteins (LDL), which often increase the risk of coronary heart disease [2,3]. Excess cholesterol can also accumulate in the liver and spleen [4]. Treatment modalities include statins, niacin and ezetimibe. First line of treatment for hypercholesterolemia is oral administration of HMG-CoA (β-hydroxy-β-methylglutaryl-CoA) reductase inhibitors, such as statins [5], which act by decreasing the LDL and increasing HDL [6]. Oral statins' administration has several disadvantages including myalgia, hepatotoxicity, and gastrointestinal disturbances such as bloating, diarrhea, and constipation [7]. The low bioavailability and extrahepatic toxicity of statins present a therapeutic challenge. Raising the dosage to address the low bioavailability is not feasible due to side effects that reduce the patient's quality of life and compliance. The current goal is to find a way to enhance drug delivery to target

tissue/cells while minimizing extrahepatic toxicity. Owing to the side effects, new options must be sought to deliver statins through alternate routes, for example the transdermal route. Although transdermal route offers a unique way to deliver drugs systemically, this route is yet to reach its full potential [8].

The skin is anatomically divided into epidermis, dermis, and the hypodermis [9]. The stratum corneum, which is the outermost layer of the epidermis, acts as body armor against hostile environmental factors including pathogens and pollutants, ultraviolet radiation and modulate moisture loss from the body [10]. For drugs to penetrate through the stratum corneum, they must bear physicochemical properties in an ideal range that permits diffusion of drugs across the skin. These include partition coefficient (logP) value between 2 and 3, molecular weight less than 500 Da, low dosage requirements usually less than 20 mg, an aqueous solubility of >1 mg/mL, and a melting point of <200 °C [11]. Moreover, drug delivery through skin requires specialized vehicles that can reversibly reduce the barrier properties of stratum corneum and allow for drug penetration through the skin to demonstrate its pharmacological actions [12]. Once such vehicle is nanoemulsion, which consists of very tiny droplets of one liquid that is dispersed in the other liquid, typically in the nanometer size range. Nanoemulsions have potential applications in transdermal drug delivery, which involves the delivery of drugs through the skin. The small droplet size of nanoemulsions allows for greater penetration through the skin, which can improve the bioavailability of certain drugs. Additionally, nanoemulsions can be formulated to target specific cells or tissues within the skin [13]. Natural oils have been routinely used to formulate nanoemulsions due to their safety and ease of availability [14]. Many studies have been reported on the use of natural oil-based nano- and micro-emulsions for the delivery of various drugs through the skin for topical and transdermal applications [15,16]. Grapeseed oil is a rich source of polyunsaturated fatty acids, namely oleic acid (15.8%) and linoleic acid (69.6%) [17] in addition to vitamin E and phenolic compounds [18]. Linoleic and oleic acid are C_{18}-fatty acids found in grapeseed oil are also an integral part of the human skin, and are major contributors in enhancing skin permeability for both lipophilic and hydrophilic APIs [19,20] without causing skin irritation.

We have recently reported a viable delivery option for a series of statins using apricot kernel oil-based nanoemulsions (NEs) and nanoemulgels (NGs) through transdermal port [21]. Results revealed that selected statins could permeate across the human skin from NEs and NGs. The current study is focused on developing NE and NG formulations using grapeseed oil for the transdermal delivery of a series of statins with the aim to correlate skin permeation with their physicochemical properties.

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DEPARTMENT OF PHAYSICS

1. Mustafa, H., Irfan, M., Sattar, A., Amjad, R. J., Latif, H., Usman, A., ... & Qin, S. (2023). First principle study of multilayered graphene/MoS2 heterostructures for photodetectors. Materials Science and Engineering: B, 289, 116205.

ABSTRACT:

Graphene/MoS_2 based heterostructures are one of the most promising candidates for future electronic and optoelectronic devices due to their unique electronic and optical properties. Here, we systematically constructed atomically thin graphene/MoS_2, graphene/MoS_2/graphene, and graphene/MoS_2/graphene/MoS_2/graphene heterostructures and performed comprehensive Density Functional Theory calculations to explore their electronic and optical properties, where GGA and HSE06 functionals were employed to explain electron transfer mechanism. Our results revealed the band gap of multilayered MoS_2/graphene narrows at K point in Brillouin zone, and can be tuned for up to 36.3 meV. Furthermore, the absorption properties of those heterostructures are the exceptional from visible to ultraviolet region, making the multilayered graphene/MoS_2 based heterostructures ideal candidate for photodetectors and optoelectronic applications.

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2. Nawaz, M., Shaikh, H., Buledi, J. A., Solangi, A. R., Raza, R., & Maher, B. (2023). Microwave-assisted synthesis of cadmium/reduced graphene oxide composite: an operative platform for highly specific electrochemical determination of bisphenol-A. Journal of Applied Electrochemistry, 53(4), 751-764.

ABSTRACT:

Environmental contamination has been a major source of concern for the world in recent decades. Pollutants in the environment are harmful entities that can cause severe diseases and pose a serious threat to the ecosystem. As a result, it becomes compulsion for modern researchers to develop such remarkable sensors that are capable of detecting contaminants in aqueous environment. In order to develop a sensitive and selective sensor for the targeted determination of Bisphenol-A (BPA), an endocrine-disrupting compound, a very efficient Cd/rGO composite was synthesized through a green microwave-assisted route. The prepared Cd/rGO composite was characterized by different analytical tools, e.g. XRD, EDX, FTIR and SEM, to study phase structure, elemental composition, functionalities, and sheets morphology, respectively. To evaluate the sensing properties of fabricated sensing material glassy carbon electrode was modified and resulting Cd/rGO/GCE was initially electrochemically characterized using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (ESI). At optimized conditions such as scan rate of 70 mV/s, PBS electrolyte of pH 7, potential window in the range of 0.0–0.9 V vs Ag/AgCl; the fabricated Cd/rGO/GCE-based sensor showed the outstanding response for BPA. Under the linear concentration range from 5 to 110 µM, the LOD and LOQ were calculated as 0.041 and 0.13 µM, respectively. Moreover, the analytical applicability of the proposed sensor was tested in different water samples, which revealed acceptable recovery values from 91.1 to 101.1%. The comprehensive experimental studies witness the reliability of

the proposed method and confirm that it could be a promising electrochemical sensor to be used at the commercial level.

Web URL: https://link.springer.com/article/10.1007/s10800-022-01797-5

3. Masood, A., Hanif, H., Ramay, S. M., Hassan, M. U., Akhtar, S., Rehman, A. R., ... & Razaq, A. (2023). Development of cerium and natural fibers freestanding composite electrodes for modern bendable energy storage applications. *Journal of Materials Research and Technology*, *23*, 2219-2230.

ABSTRACT:

Flexible and environmentally safe electrodes are high in demand for modern energy storage devices. This study reports the fabrication of cerium oxide (CeO_2) and cerium oxide-manganese oxide nanoparticles ($Ce_{0.98}$ $Mn_{0.02}$ O_2 NPs) via co-precipitation synthesis technique and further development of bendable paper-based energy storage electrodes by employing lignocelluloses fibers as binder, extracted from self-growing plant, Monochoria Vaginalis. The structural and optical properties of the prepared products are carried out by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). XRD study reveals that Mn ions are incorporated into the CeO_2 lattice to synthesize the $Ce_{0.98}$ $Mn_{0.02}$ O_2 nanoparticles. SEM/EDX and TEM/SAED are performed for surface morphological analysis and successful composite formation of CeO_2/LC and $Ce_{0.98}$ $Mn_{0.02}O_2$/LC sheets. Electrochemical measurements of CeO_2/LC and $Ce_{0.98}$ $Mn_{0.02}O_2$/LC composite sheets were performed where fabricated sheets were employed as freestanding working electrode in 2 M KOH electrolyte. CeO_2/LC and $Ce_{0.98}$ $Mn_{0.02}O_2$/LC composite sheets have shown specific capacitances of 401.5 and 544 F/g, respectively from three electrode cyclic voltammetry (CV) measurements. 2-electrodes galvanostatic charge–discharge (GCD) measurements were performed in symmetric cell which reveal the capacitance of 436 F/g and 560 F/g for CeO_2/LC and $Ce_{0.98}$ $Mn_{0.02}O_2$/LC composite paper sheets, respectively. The $Ce_{0.98}$ $Mn_{0.02}O_2$/LC (1:1) composite paper sheet shows the capacitance retention stability up to 80% after 1000 cycles at applied current density of 3.3 A/g. It can conclude that the fabricated paper electrodes can employ as working electrodes in modern energy storage devices having dual advantages of flexible and environmentally safe characteristics in the absence of any synthetic substrate/binder.

Web URL: https://www.sciencedirect.com/science/article/pii/S2238785423001448

4. ur Rehman, A., Ahmad, M., Hassan, S., Hussain, S. Q., Iqbal, M. W., & Ali, H. E. (2023). Ba substituted SrFe2O4 (SrBa0. 3Fe1. 7O4) for the removal of fluoride ions (F− 1) from the drinking water. Materials Chemistry and Physics, 295, 127165.

ABSTRACT:

Current study investigates hydrothermally prepared $SrBa_{0.3}Fe_{1.7}O_4$ for the adsorption of fluoride ions (F^{-1}) from drinking water. X-ray diffraction patterns show given sample has a single-phase

spinel structure. Scanning electron microcopy confirmed nano-sized particles in the range 12–15 nm. Fourier transform infrared spectroscopy results indicate presence of small absorption peaks due to low temperature sintering and useful elastic parameters have been analyzed as well. The Magnetic Hysteresis was measured by using Vibrating sample magnetometer between -9KOe to 9 KOe. The results revealed the soft magnetic behavior. Prepared ferrites have been investigated for time dependent and isothermal adsorption models. Pseudo second order and Temkin isotherm model best fitted the experimental results. Finally, these ferrites have been used to remove the fluoride ions from different drinking water sources in Lahore and have shown promising results.

Web URL: https://www.sciencedirect.com/science/article/pii/S0254058422014717

5. Tariq, M., Shaari, A., Chaudhary, K., Ahmed, R., Jalil, M. A., & Ismail, F. D. (2023). Magnetoelectric, and dielectric based switching properties of co-doped BiFeO3 for low energy memory technology: A first-principles study. Physica B: Condensed Matter, 650, 414489.

ABSTRACT:

First-principles calculations are carried out to grow half-metallicity, tune dielectric and magnetoelectric properties of pure and doped bismuth ferrite $BiFeO_3$ (BFO) with lanthanum (La) at A-site and cobalt (Co) at B-site as mono- and co-dopants. These calculations are performed in the Cambridge Serial Total Energy Package (CASTEP) code using ultra-soft pseudopotential (USP). A large band gap has been observed in the pure rhombohedral phase. The Co impurity atom is more favorable to decrease the band gap while La pushes the BFO towards half-metallic behavior, which develops 100% polarization in all doped BFO systems. From the dielectric response of BFO, high spin current density <s> of 8.7×10^3 A/m^2 and charge current density (j) of 6.3 × 10–11 A/m2 have been observed in the La doped system. In the case of magnetic properties, the strong magnetization (M) 32.13 MA/cm^2 and the large magnetoelectric coupling coefficient of 6.72×10^{-6} s/m have been observed in co-doped BFO.

Web URL: https://www.sciencedirect.com/science/article/pii/S0921452622007748

6. Amin, N., Atiq, A., Ikram, M., Atiq, M., Naeem, H., Yousaf, M., ... & Akbar, A. (2023). Dosimetric analysis of Rapid Arc (VMAT) treatment planning in head and neck cancer for quality assurance treatment. Journal of King Saud University-Science, 35(2), 102476.

ABSTRACT:

The current investigation aimed to compare the treatment plans of simultaneous integrated boost (SIB) fixed intensity modulated radiation therapy (IMRT) and SIB RapidArc (RA) using a number of dosimetric indices. In this study, 29 patients of nasopharyngeal carcinoma (NPC) were considered for treatment plan evaluation of SIB RA and SIB IMRT. The plans were

evaluated using conformity index (CI), target coverage (TC), gradient index (GI), external volume Index (EI), homogeneity index (HI), dose heterogeneity index (DHI), standard deviation (SD), and unified dosimetric index (UDI). The dose of each planned target volume (PTV) and organs at risk (OARs) was determined using their respective mean and median doses. In accordance with the results, there is no noticeable difference in the values of CI, TC, GI, EI, and UDI for SIB RA and SIB IMRT. DHI of PTV 54 is better for SIB IMRT as compared to SIB RA and DHI of PTV 60, PTV 70 is same for both techniques. HI, SD and sparing of OARs results in better values for SIB RA as compared to SIB IMRT. However, PTV 54 and PTV 60′s doses indicate over dosage. The dose of PTV 70 is found to be within the limits of prescribed dose for both SIB RA and SIB IMRT. SIB RA homogeneity, sparing of OAR, and SD are observed to be superior to SIB IMRT. In the case of RA, less time and a monitor unit are used. In conclusion, SIB RA is thought to be better than SIB IMRT for the treatment of NPC.

Web URL: https://www.sciencedirect.com/science/article/pii/S1018364722006577

7. ur Rehman, A., Batool, Z., Ahmad, M., Iqbal, M. W., ul Haq, A., & Hegazy, H. H. (2023). Impact of ZnO on structural and electrochemical properties of silver spinel ferrites for asymmetric supercapacitors. Journal of Electroanalytical Chemistry, 931, 117206.

ABSTRACT:

Supercapacitors are receiving great scientific attention as energy storage devices due to their rapid charge/discharge rates, high power densities, and high stability. Silver spinel ferrite ($AgFe_2O_4$) and its composites $AgFe_2O_4$@ZnO (5 & 10 %) have been synthesized by using the hydrothermal method. XRD showed that the prepared samples have a cubic spinel structure. The crystallite sizes of the samples vary from 20 to 27 nm. TEM results showed that all ferrite particles had a spherical morphology. In the UV–vis absorption spectrum, the estimated Eg was 4.9 eV for $AgFe_2O_4$ and Eg increased with higher ZnO concentration. The specific capacity for $AgFe_2O_4$@10 %ZnO is 585.4 C/g which is higher than 497 C/g for $AgFe_2O_4$@5%ZnO and 394.2 C/g for $AgFe_2O_4$. For making an asymmetric device $AgFe_2O_4$@10 %ZnO//AC, activated carbon was chosen as the negative electrode and $AgFe_2O_4$@10 %ZnO as the positive electrode. With this device, a specific capacity of 171.3 C/g was attained. AgFe2O4@10 %ZnO was found to have a power density of 720 W/kg and an energy density of 28 Wh/kg. This work indicates that a mixture of silver spinel ferrite composite ($AgFe_2O_4$@10 %ZnO) may be a more suitable electrode material for supercapacitor applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S1572665723000668

8. Aziz, M. H., Shaheen, F., Ahmad, R., Khan, A., Sharif, S., Fahad, H. M., & Huang, Q. (2023). Facile hydrothermal synthesis of NGO/NiWO3/PANI nanocomposite for durable and high performance hybrid supercapacitors. Materials Letters, 333, 133658.

ABSTRACT:

Hybrid supercapacitors signify a potential candidate for highly stable energy storage devices because of their excellent power density, low cost, and inherent safety. Hydrothermal method was used to synthesize NGO (Nitrogen doped graphene oxide)/$NiWO_3$ (nickel tungstate)/PANI (polyaniline)) nanocomposite (NC). GCD analysis offers noticeable enhanced specific capacitance of 1380 F/g as compared to $NiWO_3$ (670 F/g) and displays the cycle stability for 10 000 cycles with 92.6 % retention of capacitance at the current density of 0.5 A/g, and also shows a high energy density of 47.8 W h kg^{-1}. These obtainable outcomes propose that NGO/$NiWO_3$/PANI can be considered an efficient electrode for highly stable supercapacitors.

Web URL: https://www.sciencedirect.com/science/article/pii/S0167577X22020134

9. Khan, A., Shaheen, F., Roman, M., Ahmad, R., Mehboob, K., & Aziz, M. H. (2023). Highly redox active mesoporous Ni/Co-organic framework as a potential battery type electrode material for high energy density supercapattery. Journal of Energy Storage, 58, 106317.

ABSTRACT:

Designing potential electrochemically active metal-organic-framework (MOF) electrode materials with controllable structure and versatile nano-geometries are very pivotal to enable the forthcoming generation electrochemical energy storage systems. Among the hydrothermally synthesized materials; Nickel/MOF (NiMOF), Cobalt/MOF (CoMOF) and Nickel-Cobalt/MOF (Ni/CoMOF) with 1:1 of Ni/Co, the binary Ni/CoMOF shows excellent electrochemical performance compared to NiMOF and CoMOF, achieving a distinguished specific capacity of 594.24C g^{-1} at current density of 1 A g^{-1} in 3-electrode setup with 67.32 % remarkable rate capability at 10 A g^{-1} and excellent cyclic durability of 92.7 % after undergoing 5000 charge-discharge cycles. Further, Ni/CoMOF is employed as a positive active electrode material with Activated-carbon (Act C) and reduced-graphene oxide (rGO) sequentially as negative capacitive type electrode materials to fabricate supercapattery devices. The high cyclically stable and novel Ni/CoMOF||rGO supercapattery unveils a striking specific capacity of 307.45C g^{-1} contrary to 222C g^{-1} of Ni/CoMOF||Act-C at 1 A g^{-1} and exhibits significantly increased energy density of 66.2 Wh kg^{-1} at power density of 775.13 kW kg^{-1}. Overall, this synergy of Ni/CoMOF coupled with rGO in a hybrid configuration shows favorable energy storage features to fulfill the soaring renewable energy demands to power the digital world.

Web URL: https://www.sciencedirect.com/science/article/pii/S2352152X22023064

10. Khokhar, M. Q., Hussain, S. Q., Kim, Y., Dhungel, S. K., & Yi, J. (2023). A novel passivating contact approach for enhanced performance of crystalline silicon solar cells. Materials Science in Semiconductor Processing, 155, 107231.

ABSTRACT:

Passivated contacts based on ultrathin silicon oxide (SiO_x) layers and phosphorus-doped nanocrystalline silicon oxide (nc-SiO_x(n)) layers have been examined for their application in tunnel oxide-passivated contact (TOPCon) solar cells. Passivated contact nc-SiO_x(n)/SiO_x, is accomplished by implementing a thermally grown SiO_x tunnel layer and a plasma-enhanced chemical vapor deposited (PECVD)-grown nc-SiO_x(n) layer, which are subsequently transformed into a more crystalline phase by annealing at a higher temperature. In this research, a 3.2 × 3.2 cm solar cell was fabricated, where the base material was n-type crystalline silicon (c-Si(n)), and an aluminum oxide (Al_2O_3) acts as a passivation layer which helps to enhanced the passivation properties and indium tin oxide (ITO) layer was used on the front side, which could serve as an anti-reflection coating (ARC), respectively. The influence of the temperature, doping level, and thickness of nc-SiO_x(n) on the surface passivation of the contacts was investigated. Superior recombination current density (J_o) values of up to 2.9 fA/cm^2 were assessed for the nc-SiO_x(n)/SiO_x contacts. TOPCon solar cells with top boron-doped emitter, Al_2O_3, and ITO/rear stack of nc-SiO_x(n)/SiO_x passivation contacts were formed and resulted in V_{oc} = 650 mV and FF = 78%. Furthermore, we focused on ameliorating the achievements of solar cells using a transparent passivating contact-based nc-SiO_x(n), as well as the passivation process and operating principle.

Web URL: https://www.sciencedirect.com/science/article/pii/S1369800122007570

11. Tariq, M., Shaari, A., Chaudhary, K., Ahmed, R., Jalil, M. A., & Ismail, F. D. (2023). Computational study of switching properties in Mn and transition metal co-doped BFO. Physica B: Condensed Matter, 652, 414650.

ABSTRACT:

The coupling between electric polarization and magnetization in single-phase bismuth ferrite $BiFeO_3$ (BFO) has a potential for low-power devices. To improve the switching ability of bismuth ferrite, the effect of lanthanum (La) at A-site, and manganese (Mn) at B-site as mono- and co-dopants on spin electronic properties, spin polarization, and spin magnetic properties of $Bi_{0.75}La_{0.25}Fe_{0.75}Mn_{0.25}O_3$ in cubic phase have been explored by using the first principles. An upsurge in the density of states is detected in the inclusion of Mn and La atoms, which modify the band gap in the spin-down state. Enhancement in the magnetic moment is observed on doping of Mn and La atoms in BFO as mono- and co-dopant due to the combined involvement of these impurities to terminate the cycloidal spin structure and activate the hidden spin. The switching properties such as linear Edelstein effect and spin polarization of co-doped BFO material enhanced to 1.612 × 10^{-9} m/V and 100% respectively whereas the high value of 2.161 × 10^{-11} (A/m^2) spin current density, 3.600 × 10^{-2} (Sm^{-1}) conductivity, and 9.200 × 10^{-11} (A/m^2) charge current density have been detected in La-doped system.

Web URL: https://www.sciencedirect.com/science/article/pii/S0921452623000170

12. Ahmad, M. A., Ahmad, K., Li, H., Gassoumi, A., Raza, R., Saleem, M., ... & Abbas, G. (2023). Synergistic electrochemical properties of graphene incorporated LCZ-oxide cathode for low temperature solid oxide fuel cell. Crystals, 13(3), 434.

ABSTRACT:

Mixed metallic oxides are getting increasing attention as novel electrode materials for energy conversion devices. However, low mixed ionic-electronic conductivity and high operating temperature hamper the practical applications of these devices. This study reports an effective strategy to improve the conductivity and performance of the fuel cell at low temperature by partially incorporating graphene in the $Li_{0.1}Cu_{0.2}Zn_{0.7}$-oxide (LCZ) composite. The proposed cathode material is synthesized via the cost effective conventional solid-state route. Graphene incorporated LCZ shows excellent performance, which is attributed to the favorable charge transport paths offering low area-specific resistance. An X-ray diffractometer (XRD) and scanning electron microscope (SEM) are employed for microstructural and surface morphological analyses, respectively. Electrical conductivities of all the materials are determined by the DC four probe method, and interestingly, LCZ-1.5% graphene exhibits an excellent conductivity of 3.5 S/cm in air atmosphere at a temperature of 450 °C with a minimum value of 0.057 Ωcm^2 area-specific resistance (ASR) that demonstrates significantly good performance. Moreover, the three-layer fuel cell device is fabricated using sodium carbonated $Sm_{0.2}Ce_{0.8}O$ (NSDC) as an electrolyte, which can operate at low temperatures exhibiting open circuit voltage 0.95 V and shows a peak power density, i.e., 267.5 mW/cm^2 with hydrogen as the fuel.

Web URL: https://www.mdpi.com/2073-4352/13/3/434

13. Aziz, M. H., Khan, A., Fahad, H. M., Shaheen, F., Ahmad, R., Mehboob, K., & Huang, Q. (2023). NiZrSe3/rGO modulated porous architecture for hybrid featured asymmetric supercapacitors. Journal of Energy Storage, 63, 106982.

ABSTRACT:

Designing transition metallic chalcogenides with rGO as a potential porous platform for growth are vital to upsurge the electrochemical energy storage capabilities of supercapacitors' electrodes. This work reports hydrothermally prepared agglomerated $NiZrSe_3$ nanoparticles and a porous $NiZrSe_3$/rGO, where the latter exhibits superior charge storage properties. In comparison to $NiZrSe_3$ with specific capacitance (C_s) of 1415.7 F/g, the porous modulated material $NiZrSe_3$/rGO delivers an exceptional C_s of 2750.8 F/g at current density of 2 A/g in the 3-electrode setup. Due to its the outstanding electrochemical performance, $NiZrSe_3$/rGO is employed as a redox featured electrode material, and further integrated with activated carbon

(Act C) as a capacitive featured electrode material to construct a hybrid asymmetric supercapacitor with widened potential window and enhanced energy density. The constructed asymmetric supercapacitor unveils a specific capacitance of 140.77 F/g at current density of 1.2 A/g and rate capability of 53.6 % at 7 A/g while functioning stably under the potential range of 0–1.65 V. Moreover, it achieves extremely high energy density of 53.22 Wh/kg at power density of 990 W/kg with its long-life span in regard to cyclic stability of 80.31 % after 10,000 charging-discharging cycles. In general, this work illustrates the significance of $NiZrSe_3$/rGO as a highly redox active cathode material in hybrid featured asymmetric supercapacitors for future renewable energy storage systems.

Web URL: https://www.sciencedirect.com/science/article/pii/S2352152X23003791

14. Rafaqat, M., Ali, G., Ahmad, N., Jafri, S. H. M., Atiq, S., Abbas, G., ... & Raza, R. (2023). The substitution of La and Ba in X0. 5Sr0. 5Co0. 8Mn0. 2O3 as a perovskite cathode for low temperature solid oxide fuel cells. Journal of Alloys and Compounds, 937, 168214.

ABSTRACT:

Here we report the synthesis of La and Ba substituted $X_{0.5}Sr_{0.5}Co_{0.8}Mn_{0.2}O_3$ using sol–gel auto-combustion method and their investigation as a low temperature solid oxide fuel cell. Structural investigations revealed that $La_{0.5}Sr_{0.5}Co_{0.8}Mn_{0.2}O_3$ (LSCM) crystallized out in rhombohedral perovskite structure while $Ba_{0.5}Sr_{0.5}Co_{0.8}Mn_{0.2}O_3$ (BSCM) has hexagonal perovskite structure. Morphological analysis confirmed the porous structure with uniform distribution of grains. However, agglomeration is decreased when La is replaced with Ba. The existence of all constituent elements as per their stochiometric ratio is evaluated through energy dispersive X-ray spectroscopy. Maximum conductivity value obtained at 600 °C for LSCM and BSCM is 3.51 Scm^{-1} and 2.26 Scm^{-1}, respectively. In addition, the maximum values of current density and power density achieved by LSCM are 808 $mAcm^{-2}$ and 277 $mWcm^{-2}$ while that of BSCM are 663 $mAcm^{-2}$ and 186 $mWcm^{-2}$, respectively at low operating temperature of 600 °C. Furthermore, the open circuit voltage (V_{OC}) of LSCM and BSCM based fuel cells is 0.87 V and 0.72 V, respectively which indicates that there are minimal activation losses in the cells. These results showed that the fuel cell based on LSCM cathode has significantly higher values of power density and V_{OC} than that of BSCM based fuel cell. Therefore, LSCM based fuel cell are potential candidate for low temperature futuristic solid-state devices.

Web URL: https://www.sciencedirect.com/science/article/pii/S0925838822046059

15. Ngantchou, H. J. M., Raza, R., Nforna, E. A., Ngolui, J. L., & Sherazi, T. A. (2023). Synthesis of transition metal doped lanthanum silicate oxyapatites by a facile co-precipitation method and their evaluation as solid oxide fuel cell electrolytes. RSC advances, 13(18), 12285-12294.

ABSTRACT:

Transition metal doped apatite $La_{10}Si_{6-x}Co_xO_{27-\delta}$ (x = 0.0; 0.2; 0.8) and $La_{10}Si_{5.2}Co_{0.4}Ni_{0.4}O_{27-\delta}$ are synthesized by co-precipitation method followed by sintering. The precursor precipitates and apatite products are characterized by XRD, FTIR, TGA/DTA, Raman Spectroscopy, SEM-EDX and electrochemical impedance spectroscopy. The presence of apatite phase with hexagonal structure is confirmed through the XRD results. The conductivity measurements of the samples sintered at 1000 °C show that the ionic conductivity increases with increasing content of Co^{2+} doping into apatite that is further increased by co-doping of Ni^{2+}. The Co doped apatite ($La_{10}Si_{5.2}Co_{0.8}O_{27-\delta}$) exhibited conductivity of 1.46×10^{-3} S cm^{-1} while Co–Ni co-doped sample ($La_{10}Si_{5.2}Co_{0.4}Ni_{0.4}O_{27-\delta}$) exhibited highest conductivity of 1.48×10^{-3} S cm^{-1}. The maximum power density achieved is also for Co, Ni co-doped sample i.e., 0.65 W cm^{-2} at 600 °C. The results represented show that Co and Ni enhances the SOFC performance of apatite and makes it potential electrolyte candidate for solid oxide fuel cell application.

Web URL: https://pubs.rsc.org/en/content/articlehtml/2023/ra/d2ra07088j

16. Chavan, G. T., Kim, Y., Khokhar, M. Q., Hussain, S. Q., Cho, E. C., Yi, J., ... & Jeon, C. W. (2023). A brief review of transparent conducting oxides (TCO): the influence of different deposition techniques on the efficiency of solar cells. Nanomaterials, 13(7), 1226.

ABSTRACT:

Global-warming-induced climate changes and socioeconomic issues increasingly stimulate reviews of renewable energy. Among energy-generation devices, solar cells are often considered as renewable sources of energy. Lately, transparent conducting oxides (TCOs) are playing a significant role as back/front contact electrodes in silicon heterojunction solar cells (SHJ SCs). In particular, the optimized Sn-doped In_2O_3 (ITO) has served as a capable TCO material to improve the efficiency of SHJ SCs, due to excellent physicochemical properties such as high transmittance, electrical conductivity, mobility, bandgap, and a low refractive index. The doped-ITO thin films had promising characteristics and helped in promoting the efficiency of SHJ SCs. Further, SHJ technology, together with an interdigitated back contact structure, achieved an outstanding efficiency of 26.7%. The present article discusses the deposition of TCO films by various techniques, parameters affecting TCO properties, characteristics of doped and undoped TCO materials, and their influence on SHJ SC efficiency, based on a review of ongoing research and development activities.

Web URL: https://www.mdpi.com/2079-4991/13/7/1226

17. Mohsin, M., Farhan, S., Ahmad, N., Raza, A. H., Kayani, Z. N., Jafri, S. H. M., & Raza, R. (2023). The electrochemical study of Ni x Ce 1− x O 2− δ electrodes using natural gas as a fuel. New Journal of Chemistry, 47(18), 8679-8692.

ABSTRACT:

Solid oxide fuel cells (SOFCs) enable the direct electrochemical conversion of hydrocarbon-based fuels, such as natural gas, to electricity with high efficiency. Nevertheless, the direct utilization of natural gas in the presence of Ni-based anodes is still challenging as it causes severe deposition of carbon (coke). An excellent doping matrix is the ceria (CeO_2), which can lose oxygen without altering its structure. In this study, $Ni_xCe_{1-x}O_{2-\delta}$, where x = 0.2, 0.4, 0.6 or 0.8, is prepared using a sol–gel technique. The XRD results confirm the cubic structure of the prepared samples. The SEM analysis shows the porous and inhomogeneous nature of the particles with calculated sizes from ∼22.83 to ∼119 nm. The FTIR verifies the presence of nitrates in all the prepared anodes. UV-Vis spectroscopy demonstrates that the bandgap and optical constants decrease with increasing Ni content up to x = 0.6. The thermodynamic parameters of Ni oxidation and carbon formation are employed to study the reforming of natural gas in a SOFC system. Among the four samples, $Ni_{0.6}Ce_{0.4}O_{2-\delta}$ possesses the highest electronic conductivity (∼5.97 S cm^{-1}) at 650 °C and a low activation energy of ∼0.120 eV, which indicates good catalytic activity with enhanced electrochemical performance for the SOFC. A maximum power density of ∼386 mW cm^{-2} is obtained for NDC3 at 600 °C, which is comparable to those of other prepared electrodes. The electrochemical impedance spectrum (EIS) of NDC3 was also analysed in a hydrogen atmosphere at 600 °C. Thus, Ni-doped ceria can be considered a potential anode material for SOFCs due to its efficient and excellent catalytic properties, ease in redox-based reactions, and improved resistance against the formation of coke.

Web URL: https://pubs.rsc.org/en/content/articlelanding/2023/nj/d3nj00316g/unauth

18. Sajid Rauf , Zuhra Tayyab, Xiaofang Pan , Yatao Yang , Arshad Hussain, Hua Yunzhi, Naima Amin, Sana Rauf, Adil Saleem, Wei Xu. Highly Electroactive Sb-Doped $BaSrFeO_{3-\delta}$ Semiconductor as a Label-Free Electrochemical Aptsensing Platform for Thrombin Detection

ABSTRACT:

Thrombin plays a crucial role in regulating normal hemostatic function and various internal body processes but is rarely detected in vivo because anticoagulant substances in the blood can quickly neutralize it after early-stage coagulation. In this article, we designed a novel perovskite semiconductor Ba $_{{0}.{5}}$ Sr $_{{0}.{5}}$ FeO $_{{3}-\delta }$ by a one-step hydrothermal method as a sensing platform maintaining electroactive characteristics that can be used to conjugate the bio-recognition of aptamers and auto-probing of binding events for highly sensitive thrombin detection. In particular, the introduction of 10% Sb-dopant into Ba $_{{0}.{5}}$ Sr $_{{0}.{5}}$ FeO $_{{3}-\delta }$ semiconductor to tune the energy band structure for fast transport of charged species. Further, the synthesized Ba $_{{0}.{5}}$ Sr $_{{0}.{5}}$ SbxFe1.0-xO3-δ (${x}={0}$ –0.1) materials are physically characterized via XRD, FE-SEM, HR-TEM assisted by EDS, XPS, UV-Vis, and UPS. Moreover, aptamer plays a

key role in amplifying the electrical signal, where the prepared BaSrSb $_{{0}.{1}}$ Fe $_{{0}.{9}} 0_{{3}-{\delta }}$ particles show dispersion and aggregation upon binding with aptamers and target analyte thrombin, respectively, thereby increasing the sensitivity of the aptasensor. The electrostatic forces are responsible for making it complex between aptamers and particles, while conformational changes in aptamers pursue biomolecular binding of aptamer with thrombin. Accordingly, the electrochemical aptasensor for thrombin detection shows an impressive low limit-of-detection (LOD) of 0.02 pM in a dynamic linear range (0.05 pM–0.3 nM). The proposed electrochemical aptasensor does not require special labeling of oligonucleotides or particle surface decoration.

Web URL: https://ieeexplore.ieee.org/document/10083063/authors#authors

19. Rafique, A., Rafaqat, M., Abbas, G., Naqvi, M., Ali, A., & Raza, R. (2023). Catalytically Active and Carbon-Resistive Anode Catalyst for Solid-Oxide Fuel Cells Operated at Low Temperatures (500–600° C). ACS Applied Energy Materials, 6(12), 6401-6409.

ABSTRACT:

The development of active catalysts is always challenging in the field of energy devices. In this work, Li-doped, Ni–Cu-based, and Ni-free nanocomposite anode catalysts are synthesized and studied for solid-oxide fuel cells (SOFCs) operated at a low temperature using hydrogen and biogas as fuels. The catalysts with compositions $Ni_{0.6}Li_{0.2}Cu_{0.2}$-oxide/$La_{0.2}Ce_{0.8}O_{2-\delta}$ (NLC622-LDC), $Ni_{0.2}Li_{0.2}Cu_{0.6}$-oxide/$La_{0.2}Ce_{0.8}O_{2-\delta}$ (NLC226-LDC), and $Ni_{0.0}Li_{0.2}Cu_{0.8}$-oxide/$La_{0.2}Ce_{0.8}O_{2-\delta}$ (NLC028-LDC) are synthesized using the glycerol-assisted gel combustion route (GGCR). The structural analysis revealed the cubic structure of metallic oxide materials such as NiO and CuO phases while the cubic fluorite structure of CeO_2 as an ionic oxide phase. The optical band gaps (E_g's) of anode catalysts NLC622-LDC, NLC226-LDC, and NLC028-LDC are found to be 2.08, 2.29, and 2.37 eV, respectively. Furthermore, the anode catalyst with a higher nickel concentration shows better electrical conductivity and a lower activation energy of 3.47 S cm^{-1} and 0.67 eV at 600 °C, respectively, as compared to those of a nickel-free anode catalyst with lower nickel content. The electrochemical behavior of nanocomposites is studied at 600 °C using Nyquist plots. Electrochemical impedance analysis is carried out to see the effect of hydrocarbon fuel like biogas at the anode side. Finally, the electrochemical performance of NiLiCu-LDC catalyst-based fuel cells is tested under hydrogen and biogas fuels. Overall, the fuel cell based on the NLC622-LDC anode catalyst has higher OCV and power density with both fuels, hydrogen and biogas. Therefore, NLC622-LDC is a highly catalytically active anode catalyst which demonstrated significantly better performance for SOFCs operated at a low temperature (500–600 °C) without any carbon resistance.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsaem.3c00181

20. Areeb, F., Ahsan, I., Rasheed, A., Sumera, P., & Jamil, M. (2023). Magnetosonics with Landau levels in GaAs semiconductor systems. Physica B: Condensed Matter, 663, 414968.

ABSTRACT:

The propagation of low frequency electromagnetic magnetosonic waves in a quantum magneto electron–hole plasma is investigated. Both of the semiconductor plasma species are magnetically quantized at equilibrium. The quantization is included through recoil effect and Landau effects on applying quantum hydrodynamic model (QHD). Analytical results of quantum hydrodynamical model are then verified numerically for GaAs plasma system.

Web URL: https://www.sciencedirect.com/science/article/pii/S0921452623003356

21. Siddiqui, R., Rani, M., Shah, A. A., Razaq, A., Iqbal, R., Neffati, R., & Arshad, M. (2023). Fabrication of tricarboxylate-neodymium metal organic frameworks and its nanocomposite with graphene oxide by hydrothermal synthesis for a symmetric supercapacitor electrode material. Materials Science and Engineering: B, 295, 116530.

ABSTRACT:

Efficient energy storage and delivery of electrical energy is necessary for the use of advanced electrode materials in super-capacitors, rendering their development pivotal. We employed simple and economical hydrothermal technique to synthesize Nd-metal organic frameworks (MOFs) and Nd-MOFs/GO composite and evaluated their suitability as electrode materials through comprehensive investigation. Characterizations of the synthesized materials were done by various techniques, including XRD, FTIR (using ATR method) and SEM. Based on the results obtained, it was found that the Nd-MOFs/GO composite-based electrode had a specific capacitance of 633.5 Fg^{-1} when tested at a current density of 0.3 Ag^{-1}, which is significantly higher than that of Nd-MOFs electrode (11.3 Fg^{-1}). Additionally, electrochemical impedance spectroscopy (EIS) analysis demonstrated the lowest equivalent series resistance (ESR) of 0.8 Ω for the Nd-MOFs/GO electrode. The Nd-MOFs/GO composite electrode exhibited a cyclic stability of 88.76 % after 4000 cycles and coulombic efficiency of 95.1%, when subjected to a current density of 3 Ag^{-1}. Moreover XRD showed that the synthesized hybrid exhibited an improved crystallinity of the hexagonal phase. The FTIR analysis using ATR method confirmed the presence of organic ligands and functional groups in the synthesized materials. The results of our study indicate that the Nd-MOFs/GO hybrid nanocomposite-based electrode material holds potential as a highly efficient candidate for super-capacitor applications. The reported method of synthesizing MOFs provides an effective approach to fabricate new electrode materials with excellent electrochemical characteristics.

Web URL: https://www.sciencedirect.com/science/article/pii/S0921510723002726

22. Lu, Y., Mushtaq, N., Shah, M. Y., Almutairi, B. S., Dong, Y., Yousaf, M., & Raza, R. (2023). Theoretical and experimental design for promoting the oxygen reduction activity of SrCoO3 perovskite-based cathode for PCFCs by bimetal-ions doping. International Journal of Hydrogen Energy, 48(87), 34034-34044.

ABSTRACT:

Low temperatures ceramic fuel cells (LT-CFCs) including solid oxide and proton conducting fuel cells (SOFCs/PCFCs), hold a great promise for abundant large-and small scaled realapplication. Sluggish oxygen reduction reaction (ORR) activity at lower operating temperatures hindered the development of LT-CFCs. Strontium cobalt-based perovskite-oxides (SrCoO3 d) materials have been frequently considered as a promising next-generation cathode for CFCs. Different doping stratigy are used to improve the mixed ionic (Hþ/O2-) and electronic conductivity of SrCoO3——d, which help to extend the electrochemical reaction zone for oxygen reduction. Herein, we introduced bi-metal doping of La and Ce at B-site of SrCoO3——d to produce SrCo0.8Ce0.1La0.1O3-d (SCCL) pervoskite structure for PCFCs cathode. The developed SLCC cathode exhibits ultra-low-area-specific polarization resistance of 0.11 U cm2 and large oxygen reduction reaction (ORR) response at intermediate operating temperatures. We have demonstrated power density of 510 mWcm——2 using SLCC cathode over proton conducting BaCe0.7Zr0.2Y0.1O3-d electrolyte at 600 C and even with possible operation at 450 C. The ORR activity of SLCC perovskites is found to strongly rely on the two proposed descriptors, where La and Ce doping at Co-site-in SrCoO3——d located in the auspicious zone for predicting the moderate value of vacancy formation energy and ions

Web URL: https://www.sciencedirect.com/science/article/pii/S0360319923023728

23. Bakar, A., Alrashdi, A. O., Ali, S., Rehman, S. U., Afaq, A., & Asif, M. (2023). Opto-electronic and thermoelectric properties of XMgY (X= Li, Na; Y= Al, Ga) alloys: GGA and SCAN based approaches. Materials Today Communications, 36, 106451.

ABSTRACT:

The half Heusler alloys are important class of materials which are utilized for memory as well as the spintronic devices. The thermoelectric response calculations are also reported for Heuslers alloys. In this research work, electronic dispersion curves, thermoelectric and optical parameters of XMgY (X=Li, Na/Y=Al, Ga) half Heuslers have been investigated by employing the pseudopotential approach along side the Boltzmann transport theory. The XMgY (X=Li, Na/Y=Al, Ga) were reported stable in $C1b$ type structure by energy-volume optimization, Born stability criteria on elastic constants and positive phonon modes in full zone in phonon dispersion curves by Afaq et al. Both the SCAN and Generalized Gradient Approximation proved these alloys metallic in nature. To understanding the complex phenomenon of electron flow inside a material, Fermi surfaces are studied and discussed. The different thermoelectric response parameters are computed in temperature range 300 to 1200 K. The comprehensive analysis of

imaginary part of dielectric constant predicts the utility of these alloys in sensors and opto-electronic devices.

Web URL: https://www.sciencedirect.com/science/article/pii/S235249282301142X

24. Li, J., Mushtaq, N., Shah, M. Y., Almutairi, B. S., Rauf, S., Raza, R., ... & Lu, Y. (2023). Large oxygen reduction response of CaFe2O4-WO3 heterostructure composite for protonic ceramic fuel cell cathode. Ceramics International, 49(18), 29736-29746.

ABSTRACT:

Protonic Ceramic fuel cells (PCFCs) hold great promise for many applications; however, their high operating temperature hinders their commercial use in practice. The crucial issue that limits the electrochemical performance of PCFCs (including oxygen and proton-ion-conducting) is the sluggish oxygen redox reaction (ORR) at the cathode surface at low operating temperatures. Herein, we have developed a CaFe2O4-WO3 heterostructure composite by interface-vacancy engineered for an efficient ORR electrocatalyst for LT-PCFCs. The CaFe2O4-WO3 heterostructure composite exhibits very low cathodic area-specific resistance (ASR) and high oxygen reduction reaction (ORR) activity response at low operating temperatures of 400–550 ◦C using a BaCe0.7Zr0.2Y0.1O3-δ (proton-conducting) electrolyte. We have demonstrated high-power density of 585 ± 2% mW-cm− 2 with a current density of 1660 mA-cm− 2 at 550 ◦C with H2 fuel and atmospheric air as oxidant and even with possible operation at 400 ◦C. Moreover, the CaFe2O4-WO3 heterostructure composite shows a very low proton migration energy and activation energy compared to individual CaFe2O4 and WO3, helping to promote ORR activity. Various spectroscopic measurements, such as X-ray diffraction, high resolution transmission electron microscopy (HR-TEM), U-visible spectroscopy (UV–visible), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations are employed to understand the interfacial properties for the improved ORR electrocatalytic activity of the CaFe2O4-WO3 heterostructure composite cathode. Our obtained experimental and theoretical results can further help to develop functional cobalt-free electrocatalysts for LT-PCFCs.

Web URL: https://www.sciencedirect.com/science/article/pii/S0272884223018023

25. Jabeen, Z., Dawood, A., Alomar, M., Khan, S. N., Ali, I., Asif, M., ... & Ahmad, M. (2023). Hydrothermal synthesis of nickel substituted magnesium ferrites (NixMg1-xFe2O4) and insight into the detailed structural, magnetic and electrochemical properties. Surfaces and Interfaces, 40, 103130.

ABSTRACT:

A series of single-phase nickel (Ni^{+2}) substituted magnesium Mg-spinel ferrites ($Ni_xMg_{1-x}Fe_2O_4$) were synthesized by hydrothermal technique and investigated for morphological, structural, magnetic, and electrochemical properties. Experimental characterization techniques revealed that

single-phase spinel structure was confirmed by X-ray diffraction, lattice parameter dropped with increasing Ni concentrations, nanoparticles clustered together, the nanoparticles in the SEM micrographs of different sizes are clustered together. Raman spectra showed lower wave numbers, FTIR spectrum showed that peaks move towards lower wave numbers because of nickel's substitution, and this shortens the Fe-O bond hence reduces the lattice parameter, saturation magnetization increased, coercivity decreased, specific capacitance decreased, and loop size increased. These ferrites are suitable for energy storage applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S246802302300500X

26. Asif, M., Afaq, A., Amin, M., Raouf, K., Majeed, A., & Asif, M. (2023). Optical properties of strontium titanate (STO) thin films using transfer matrix method. Materials Today

Communications, 37, 106966.

ABSTRACT:

The transfer matrix method is a very effective theoretical technique investigating the optical properties of a single and layered thin films. By utilizing the transfer matrix method, the transmission, reflection, and absorption properties of Strontium Titanate (STO) thin films are analyzed across a wide range of wavelengths. For 250 nm and 260 nm thick STO thin films, the optical direct band gaps 3.49 eV and 3.59 eV respectively are found to be consistent with the experimental findings. Additionally, the impact of film thickness and optical band gap on response of STO thin films is explored. It is noticed that with the increase in thickness of thin film, the band gap is redshifted and its value is increased as well. The findings presented in this paper contribute to a comprehensive understanding of the optical behavior of STO thin films, enabling further advancements in the design and fabrication of STO-based optoelectronic devices.

Web URL: https://www.sciencedirect.com/science/article/pii/S2352492823016574

27. Mir, A., Iqbal, M., Amjad, U. E. S., Sherin, L., & Mustafa, M. (2024). Fabrication and Performance Evaluation of Schottky Diode Device Fabricated Utilizing Ultrathin Silver Nanowires-PEDOT: PSS Composite Electrode. JOM, 76(2), 646-655.

ABSTRACT:

Printable, highly efficient and cost-effective electrodes are an essential component required for modern intelligent electronics. Here, we present the fabrication of a printed silver nanowires and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate composite electrode through the electrospray technique. Silver nanowires were synthesized in-house using the hybrid polyol method. The structural and optical behavior analyses of silver nanowires were conducted using XRD and UV-Vis spectroscopy, respectively. Optical microscopy revealed presence of defect-

free electrosprayed films while FESEM indicated presence of ultrathin (75 nm) silver nanowires. The electrical behavior of the composite electrode indicates that by the addition of silver nanowires, an increase in electrical conductivity (≈300 times) from pristine poly(3,4-ethylenedioxythiophene) polystyrene sulfonate was achieved. Moreover, a sandwich-structured diode was fabricated using the functional film electrode with polyaniline as a p-type semiconductor. The current-voltage behavior of the fabricated diode reveals the rectification behavior with a very low turn-on-voltage of 1.47 V. The conductive nature of the composite electrode indicates its proficiency as a working electrode in printed electronics.

Web URL: https://link.springer.com/article/10.1007/s11837-023-06055-3

28. Khan, S. N., Mir, A., Manzoor, S., & Raees, R. (2024). Effect of rare earth doping on the electromagnetic response of hard ferrites SrFe12O19 for potential application in high-frequency devices. Materials Chemistry and Physics, 320, 129378.

ABSTRACT:

This work explores the synthesis, characterization, and potential application of rare earth doping on hard ferrites, focusing on their unique electromagnetic properties for potential applications in radio frequency (RF) devices. This study investigates the influence of rare earth (Sm^{+3}) doping on structural and dielectric properties of strontium ferrite. Samarium doped strontium ferrite with composition $Sr_{1-x}Sm_xFe_{12}O_{19}$ *(x = 0.0,0.1,0.2,0.3)* is prepared using the sol-gel auto combustion technique. The prepared samples' crystal structural and morphological properties were studied using an X-ray diffractometer (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and RAMAN spectroscopy. XRD patterns of rare earth substituted strontium ferrite confirmed the formation of a hexagonal phase together with an impurity phase of Fe_2O_3 for *x = 0.3*. FTIR analysis establishes metal and Oxygen *(M-O)* stretching vibrations in $Sr_{1-x}Sm_xFe_{12}O_{19}$ due to various interstitial sites in its structure. The Raman result shows the presence of four Raman active modes in prepared powders. Meanwhile, the broadening of Raman peaks with Sm2+ doping is also observed. Electromagnetic properties were obtained in the frequency region 2–18 GHz. An increasing tendency is observed in the real part of permittivity and permeability of all doped samples in the frequency region 2–18 GHz. The reflection loss was observed for sample *x = 0.2* with the maximum value of > -40 dB at 18 GHz, and the adequate absorption bandwidth is 10 GHz from 8 GHz to above 18 GHz. On the basis of these results, among all prepared samples, Sr0.8Sm0.2 Fe12O19 is found to be the most suitable candidate for microwave absorbers.

Web URL: https://www.sciencedirect.com/science/article/pii/S0254058424005030

29. Rasheed, S., Latif, H., Masood, M. F. U. D., Sattar, A., Shabbir, S. A., Razaq, A., ... & Ali, S. (2023). Comparative study of 2D/3D hybrid perovskite solar cell containing different modified carbon nanomaterials based Electron Transport Layers (ETL). Optical Materials, 144, 114364.

ABSTRACT:

Charge transport facilitation in the electron transport layer is necessary for high-efficiency perovskite solar cells. Carbonaceous materials such as graphene (G) and carbon nanotubes (CNTs) have been extensively used in energy storage and conversion applications. Here we report the novel design of ETL based on the combinations of tin oxide, graphene nanoribbons, nitrogen-doped graphene nanoribbons, and gold nanoparticles for 2D/3D perovskite solar cells. Three different ETLs were employed to get three 2D/3D PSCs with novel device architectures. The effect of different ETLs on the performance of solar cells is investigated. Results reveal that due to better optical and electrical behavior, the solar cell employing a composite of tin oxide, graphene nanoribbons, nitrogen-doped graphene nanoribbons, and gold nanoparticles as ETL has attained a higher PCE of 10.77%

Web URL: https://www.sciencedirect.com/science/article/pii/S0925346723009369

30. Mustafa, H., Khan, J., Sattar, A., Irfan, M., Gul, S., & Zalfiqar, I. (2023). High-Performance Field-Effect Transistor Fabricated on CVD-Grown MoS2 Monolayers with Indium Contacts. Journal of Electronic Materials, 52(11), 7157-7163.

ABSTRACT:

Molybdenum disulfide (MoS_2), an emerging two-dimensional semiconductor material, has been keenly studied for field-effect transistors (FETs). In this work, we explored the optical and electrical properties of FETs fabricated by MoS_2 flakes grown by chemical vapor deposition (CVD) and transferred to the electrodes through propylene carbonate film. Large-area, high-quality and highly crystalline MoS_2 monolayers up to 58 µm are obtained through CVD. Flakes are characterized by optical microscopy, atomic force microscopy, Raman spectroscopy, and photoluminescence analysis. The back-gated measurements are performed in ambient conditions without any encapsulation of the device. The fabricated device reveals *n*-type behavior with high field-effect mobility of 32 cm^2/V s and high current ON/OFF ratio of 10^6. Good ohmic contact is achieved while using indium as source/drain electrodes. The large sized, highly crystalline flakes of MoS_2 and the fabricated device showing high field-effect mobility and ON/OFF ratio make them potential candidates for high-performance nanoelectronics and optoelectronics devices.

Web URL: https://link.springer.com/article/10.1007/s11664-023-10625-1

31. Khan, K. I., Sattar, A., Latif, H., Irfan, M., Usman, A., Mustafa, H., ... & Alvi, F. (2023). Effect of the Strength of Carbon Nanotube Network on the Efficiency of CNFET Based on Self-Assembled Molecular Monolayer Gate Dielectric. ACS Applied Electronic Materials, 5(12), 6660-6667.

ABSTRACT:

The current demand calls for the development of electronic devices that are efficient, compact, lightweight, and cost-effective. Researchers are striving to enhance the performance of field-

effect transistors (FETs), the fundamental components of microelectronics. However, a persistent challenge in present FETs is the trade-off between mobility and the I_{ON}/I_{OFF} current ratio, which hampers their overall performance. To address this issue, our work introduces an innovative approach to creating field-effect transistors based on single-walled carbon nanotubes (SWCNTs) combined with self-assembled monolayers (SAMs) as the gate dielectric. Three distinct SAMs, octanethiol, dodecanethiol (DDT), and benzyl mercaptoan (BMT), each with differing dielectric constants, serve as gate dielectrics in SWCNT-FETs. Our research involves a comparative analysis of the three fabricated FETs. This study explores the influence of different SAMs and carbon nanotube (CNT) surface coverage on the performance of carbon nanotube field-effect transistors (CNTFETs) based on random networks. Parameters evaluated include the on/off ratio, field-effect mobility, and subthreshold swing. Intriguingly, the research reveals that CNTFETs with lower surface coverage exhibit significantly improved characteristics compared to those of high surface coverage devices. Among the manufactured CNTFETs, the DDT sample with low surface coverage demonstrates an optimal balance between the I_{ON}/I_{OFF} current ratio and mobility. Furthermore, our findings are supported by density functional theory results, indicating that SAMs with longer chain lengths, such as DDT, and aromatic molecules, such as BMT, possess higher dielectric constants, rendering them more favorable for transistor applications.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsaelm.3c01181

32. Saleem, M., Latif, H., Anjum, D. H., Shabbir, S. A., Sattar, A., & Usman, A. (2023). Au/NG/SWCNTs/FTO-glass modified electrode based electrochemical biosensor for DNA detection. Microchemical Journal, 193, 109206.

ABSTRACT:

An easy, quick, and efficient detection of Multidrug Resistance (MDR) of cancer cells at the clinical level is the need of the hour for the effective treatment of leukemia patients. In this study, we reported carbon nanomaterials-based biosensors based on Au nanoparticles (Au-NPs) decorated on Nitrogen-doped Graphene (NG) and Single-Walled Carbon Nanotubes (SWCNTs) for effective, efficient, and sensitive detection of affected DNA. Three Au/NG/SWCNT-based Modified Electrode (ME) were made containing 2, 4, and 6 mg SWCNTs. The thiol group attached at the 5′end was immobilized at ME due to a strong bond between the Au-NPs and thiol group. NG/SWCNTs enhanced the performance of the composite due to its better sensitivity and fast electron transport. Electrochemical Impedance Spectroscopy (EIS), Cyclic Voltammetry (CV), and Differential Potential Voltammetry (DPV) analysis were performed to monitor the performance of the sensor after the hybridization of target DNA onto the capture probe on the modified electrode surface. Different target DNA sequences were used to check the selectivity and sensitivity of the fabricated biosensor. The selectivity performance of prepared DNA sensors was also proved to be good shown by DPV results. The findings of this study provide insights for developing new highly sensitive, selective, and cost-effective portable biosensors for MDR gene detection, which will enable the early diagnosis of cancer more effective at the clinical level.

Compared with previous DNA sensors with oligonucleotides directly incorporated on carbon electrodes, this carbon nanotube-based assay with its large surface area and good charge-transport characteristics dramatically increased DNA attachment quantity and complementary DNA detection sensitivity.

Web URL: https://www.sciencedirect.com/science/article/pii/S0026265X23008251

33. Jiang, Y., Fahmy, M. A., Amin, N., Sohail, A., Alam, F., & Nofal, T. A. (2023). Artificial intelligence to deal with the post COVID-19 fractal dynamics linked with economy. Fractals, 31(10), 2340002.

ABSTRACT:

Data-based studies have always provided useful insights of the research problem, provided that correct statistical modeling and inference strategies are adopted. For bi-directional studies or longitudinal datasets, it is always difficult to analyze the dependence of variables and their impact on the key features. With the advancement in the fields of data science and the applied mathematical modeling, these difficulties are well resolved. The machine learning algorithms can help to streamline the data-based studies in a robust manner. During this research, the COVID-19 data are analyzed with the aid of machine learning classification tools to identify the predictors, directly influenced by the pandemic. The impact of COVID-19 on the world's economy can be better interpreted with the aid of data-based research. The data linked to the unemployment rates, during the frequent waves of COVID-19, are extracted from different sources and analyzed during this research for better forecasting measures. The nonlinear dynamical analysis can be visualized with the aid of the 2D fractal pattern generation approach. Thus the current research is an attempt to connect the outcomes of the classification analysis to the 2D fractal generation for better visual interpretation of lengthy large datasets.

Web URL: https://www.worldscientific.com/doi/abs/10.1142/S0218348X23400029

34. Jabeen, Z., Dawood, A., Alomar, M., Khan, S. N., Ali, I., Asif, M., ... & Ahmad, M. (2023). Hydrothermal synthesis of nickel substituted magnesium ferrites (NixMg1-xFe2O4) and insight into the detailed structural, magnetic and electrochemical properties. Surfaces and Interfaces, 40, 103130.

ABSTRACT:

A series of single-phase nickel (Ni^{+2}) substituted magnesium Mg-spinel ferrites ($Ni_xMg_{1-x}Fe_2O_4$) were synthesized by hydrothermal technique and investigated for morphological, structural, magnetic, and electrochemical properties. Experimental characterization techniques revealed that single-phase spinel structure was confirmed by X-ray diffraction, lattice parameter dropped with increasing Ni concentrations, nanoparticles clustered together, the nanoparticles in the SEM micrographs of different sizes are clustered together. Raman spectra showed lower wave numbers, FTIR spectrum showed that peaks move towards lower wave numbers because of

nickel's substitution, and this shortens the Fe-O bond hence reduces the lattice parameter, saturation magnetization increased, coercivity decreased, specific capacitance decreased, and loop size increased. These ferrites are suitable for energy storage applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S246802302300500X

35. ur Rehman, A., Batool, Z., Ahmad, M., Iqbal, M. W., ul Haq, A., & Hegazy, H. H. (2023). Impact of ZnO on structural and electrochemical properties of silver spinel ferrites for asymmetric supercapacitors. Journal of Electroanalytical Chemistry, 931, 117206.

ABSTRACT:

Supercapacitors are receiving great scientific attention as energy storage devices due to their rapid charge/discharge rates, high power densities, and high stability. Silver spinel ferrite ($AgFe_2O_4$) and its composites $AgFe_2O_4$@ZnO (5 & 10 %) have been synthesized by using the hydrothermal method. XRD showed that the prepared samples have a cubic spinel structure. The crystallite sizes of the samples vary from 20 to 27 nm. TEM results showed that all ferrite particles had a spherical morphology. In the UV–vis absorption spectrum, the estimated Eg was 4.9 eV for $AgFe_2O_4$ and Eg increased with higher ZnO concentration. The specific capacity for $AgFe_2O_4$@10 %ZnO is 585.4 C/g which is higher than 497 C/g for $AgFe_2O_4$@5%ZnO and 394.2 C/g for $AgFe_2O_4$. For making an asymmetric device $AgFe_2O_4$@10 %ZnO//AC, activated carbon was chosen as the negative electrode and $AgFe_2O_4$@10 %ZnO as the positive electrode. With this device, a specific capacity of 171.3 C/g was attained. AgFe2O4@10 %ZnO was found to have a power density of 720 W/kg and an energy density of 28 Wh/kg. This work indicates that a mixture of silver spinel ferrite composite ($AgFe_2O_4$@10 %ZnO) may be a more suitable electrode material for supercapacitor applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S1572665723000668

36. ur Rehman, A., Ahmad, M., Hassan, S., Hussain, S. Q., Iqbal, M. W., & Ali, H. E. (2023). Ba substituted SrFe2O4 (SrBa0. 3Fe1. 7O4) for the removal of fluoride ions (F− 1) from the drinking water. Materials Chemistry and Physics, 295, 127165.

ABSTRACT:

Current study investigates hydrothermally prepared $SrBa_{0.3}Fe_{1.7}O_4$ for the adsorption of fluoride ions (F^{-1}) from drinking water. X-ray diffraction patterns show given sample has a single-phase spinel structure. Scanning electron microcopy confirmed nano-sized particles in the range 12–15 nm. Fourier transform infrared spectroscopy results indicate presence of small absorption peaks due to low temperature sintering and useful elastic parameters have been analyzed as well. The Magnetic Hysteresis was measured by using Vibrating sample magnetometer between -9KOe to 9 KOe. The results revealed the soft magnetic behavior. Prepared ferrites have been investigated for time dependent and isothermal adsorption models. Pseudo second order and Temkin isotherm model best fitted the experimental results. Finally, these ferrites have been used

to remove the fluoride ions from different drinking water sources in Lahore and have shown promising results.

Web URL: https://www.sciencedirect.com/science/article/pii/S0254058422014717

37. Ahmad, M., Yaseen, H., Ali, I., Rafiq, K., Hussain, S. Q., & Shehzad, K. (2023). Sol-gel Synthesis of Mn-substituted Copper Ferrite Nano Particles as Anode for Lithium Ion Batteries. Journal of Materials and Physical Sciences, 4(2), 61-72.

ABSTRACT:

Mn substituted copper ferrites (Mn x Cu 1-x Fe 2 O 4, x= 0, 0.33, 0.67, 1.00) have been synthesized from metal nitrates and citric acid by sol-gel method (chemical process). This study aims to know the effects of Mn substitution on structural, magnetic, and electrochemical properties of copper ferrites. For characterizing the prepared ferrites, different techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared (FTIR) spectroscopy were used. In addition, vibrating sample magnetometer (VSM) is used to investigate the magnetic properties such as saturation magnetization (Ms), residual magnetism (Mr) and coercive force (Hc). A single-phase spinal structure was confirmed by XRD and lattice parameter was increased from 8.36 Å to 8.52 Å with increasing Mn contents. Micrographs of SEM shows that nanoparticles are agglomerated and non-uniform in size. The FTIR analysis shows that theses absorption band about 1422 cm-1 to 1434 cm-1 was attributed octahedral B-site. For pure copper ferrite, band is shifted towards higher frequency by manganese content. The results from CV showed that the increasing in scan rate and specific capacitance decreases due to increase in the area loop which clearly means that the investigated samples are best for storage devices such as lithium ion batteries (LIBs).

Web URL: https://journals.internationalrasd.org/index.php/jmps/article/view/1981

38. Noor, F., Aziz, M. H., Shaheen, F., Ahmed, M., Ali, S. M., & Huang, Q. (2023). Architecture of GO/CoFe2O4/ZnO nanocomposite for efficient fluoride removal: an approach using RSM, ANN and GRU modeling. Surfaces and Interfaces, 43, 103583.

ABSTRACT:

The presence of fluoride in wastewater possesses a significant risk to the environment. Graphene oxide-based nanocomposites were prepared as potential adsorbents for fluoride removal from water. Various techniques including X-ray diffraction (XRD), Scanning Electron Microscopy (FE-SEM), Energy dispersive X-ray (EDX), Fourier Transform Infrared Spectroscopy (FTIR), RAMAN spectroscopy, Ultraviolet-Visible spectroscopy (UV–vis), Vibrating Sample Magnetometer (VSM), X-ray Photoelectron Spectroscopy (XPS), Brunauer Emmett Teller (BET), and Electrochemical Impedance Spectroscopy (EIS) were employed to investigate the morphological, structural, chemical composition, elemental analysis, surface area, optical band gap, etc. of the $CoFe_2O_4$, $CoFe_2O_4$/ZnO composite and GO/$CoFe_2O_4$/ZnO nanocomposite. XRD analysis confirmed a reduction in crystallite size to

15.7 nm of GO/$CoFe_2O_4$/ZnO. Batch adsorption studies were conducted for fluoride removal with input independent variables (pH, temperature, initial fluoride concentration, time, and an adsorbent GO/$CoFe_2O_4$/ZnO dosage). The Response Surface Methodology (RSM) and Gated Recurrent Unit (GRU) models predicted the fluoride removal process, with RSM achieving an optimal fluoride removal of 94.3%, GRU achieving 94.5% and Artificial neural network (ANN) attaining 93.72%. A kinetic investigation was carried out using Pseudo first order (PFO) and Pseudo second order (PSO). Results confirmed that the adsorption of fluoride followed the PSO kinetic model with an (R^2 = 0.999). Isotherm studies were conducted using Langmuir, Temkin, Freundlich, and Dubinin Radushkevich isotherms. Among them, the best model follows an adsorption mechanism, with (R^2 = 0.984) and an adsorption capacity of 10.68 mgg^{-1} was Langmuir Isotherm. The real water sample of Ravi River, Pakistan also investigated for fluoride removal capability. This research contributes to the promotion of RSM and GRU modeling with high sustainability for water purification. The contemplated nanocomposite (GO/$CoFe_2O_4$/ZnO) is a potential adsorbent for the mechanism of water detoxification containing fluoride which may be useful for environmental remediation as well.

Web URL: https://www.sciencedirect.com/science/article/pii/S2468023023009525

39. Aziz, M. H., Shaheen, F., Ahmad, R., Khan, A., Sharif, S., Fahad, H. M., & Huang, Q. (2023). Facile hydrothermal synthesis of NGO/NiWO3/PANI nanocomposite for durable and high performance hybrid supercapacitors. Materials Letters, 333, 133658.

ABSTRACT:

Hybrid supercapacitors signify a potential candidate for highly stable energy storage devices because of their excellent power density, low cost, and inherent safety. Hydrothermal method was used to synthesize NGO (Nitrogen doped graphene oxide)/$NiWO_3$ (nickel tungstate)/PANI (polyaniline)) nanocomposite (NC). GCD analysis offers noticeable enhanced specific capacitance of 1380 F/g as compared to $NiWO_3$ (670 F/g) and displays the cycle stability for 10 000 cycles with 92.6 % retention of capacitance at the current density of 0.5 A/g, and also shows a high energy density of 47.8 W h kg^{-1}. These obtainable outcomes propose that NGO/$NiWO_3$/PANI can be considered an efficient electrode for highly stable supercapacitors.

Web URL: https://www.sciencedirect.com/science/article/pii/S0167577X22020134

40. Younis, H., Shafique, S., Ehsan, Z., Ishfaq, A., Mehboob, K., Ajaz, M., ... & Muhammad, W. (2023). Radiometric examination of fertilizers and assessment of their health hazards, commonly used in Pakistan. Nuclear Engineering and Technology, 55(7), 2447-2453.

ABSTRACT:

The radioactivity concentrations of Naturally Occurring Radioactive Materials (NORM) i.e., ^{226}Ra, ^{232}Th, and ^{4}K in various chemical fertilizers being used in the agricultural soil of

Pakistan were determined utilizing gamma spectrometry by employing a High Purity Germanium (HPGe) detector. The radioactivity concentrations of ^{226}Ra, ^{232}Th, and ^{4}K extended from 2.58 ± 0.8–265.7 ± 8.8 Bq kg^{-1}, 1.53 ± 0.14–76.6 ± 1.07 Bq kg^{-1} and 36.5 ± 1.34–15606.7 ± 30.2 Bq kg^{-1} respectively. The radiological hazard parameters such as internal and external indices and annual effective dose rates were calculated, while excessive lifetime cancer risk factors for the indoor and outdoor areas were found in the range from 0.3×10^{-3} to 10.723×10^{-3} and 0.03×10^{-3} to 2.7948×10^{-3} of most fertilizers, however, some values were slightly higher than the UNSCEAR (The United Nations Scientific Committee on the Effects of Atomic Radiation) recommended values for potash-containing fertilizers such as MOP (Muriate of Potash).

Web URL: https://www.sciencedirect.com/science/article/pii/S1738573323001298

41. Ramzan, M., Rani, M., Siddiqui, R., Shah, A. A., Arshad, M., Ghauri, M. W., ... & Sillanpää, M. (2023). Synthesis and analytical characterization of Ca-BTC metal organic framework. Heliyon, 9(11).

ABSTRACT:

Metal Organic framework (MOF) has been a class of great interest during the past few years owing to its decidedly applicative, easily synthesized and improved characteristics. Ca-BTC MOF is synthesized by Hydrothermal technique and reported for the first time. Its structural morphology was analyzed using XRD, SEM, and EDS, showing the tetragonal crystal structure having grain size of 24.92 nm and purity of sample respectively. FTIR, Raman Spectroscopy ensures the metal organic framework between Calcium and the tri-carboxylic group. Photoluminescence measures the energy gap of 3.792 eV, showing approximately the semiconducting behavior of synthesized material. Zeta potential having value of −13.5 mV confirms the instability having good microbial activity and conductivity i.e 0.290 mS/cm which reveals important insights into its electrical properties.

Web URL: https://www.cell.com/heliyon/fulltext/S2405-8440(23)08522-5

42. Afroz, L., Rafaqat, M., Ahmad, M. A., Bashir, T., Naqvi, M., Abbas, G., ... & Raza, R. (2023). Nanocomposite Catalyst (1–x) NiO-x CuO/y GDC for Biogas Fueled Solid Oxide Fuel Cells. ACS Applied Energy Materials, 6(21), 10918-10928.

ABSTRACT:

The composites of Ni–Cu oxides with gadolinium doped ceria (GDC) are emerging as highly proficient anode catalysts, owing to their remarkable performance for solid oxide fuel cells operated with biogas. In this context, the nanocomposite catalysts $(1 - x)$NiO-xCuO/yGDC (x = 0.2–0.8; y = 1,1.3) are synthesized using a solid-state reaction route. The cubic and monoclinic structures are observed for NiO and CuO phases, respectively, while CeO_2 showed cubic fluorite structure. The scanning electron microscopic images revealed a rise in the particle size with an

increase in the copper and GDC concentration. The optical band gap values are calculated in the range 2.82–2.33 eV from UV–visible analysis. The Raman spectra confirmed the presence of vibration modes of CeO_2 and NiO. The electrical conductivity of the nanocomposite anodes is increased as the concentration of copper and GDC increased and reached at 9.48 S cm^{-1} for 0.2NiO-0.8CuO/1.3GDC composition at 650 °C. The electrochemical performance of (1 – *x*)NiO-*x*CuO/*y*GDC (*x* = 0.2–0.8; *y* = 1,1.3)-based fuel cells is investigated with biogas fuel at 650 °C. Among all of the as-synthesized anodes, the fuel cell with composition 0.2NiO-0.8CuO/1.3GDC showed the best performance, such as an open circuit voltage of 0.84 V and peak power density of 72 mW cm^{-2}. However, from these findings, it can be inferred that among all other compositions, the 0.2NiO-0.8CuO/1.3GDC anode is a superior combination for the high electrochemical performance of solid oxide fuel cells fueled with biogas.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsaem.3c01683

43. Mehran, M. T., Khan, M. Z., Song, R. H., Lim, T. H., Naqvi, M., Raza, R., ... & Hanif, M. B. (2023). A comprehensive review on durability improvement of solid oxide fuel cells for commercial stationary power generation systems. Applied Energy, 352, 121864.

ABSTRACT:

Solid oxide fuel cells (SOFCs) are recognized as an alternative for power generation applications due to their high efficiency and environment-friendly behaviour. The electronic devices and power age could be revolutionized with the commercialization of such devices. Stationary power generation systems based on SOFCs are a step closer to commercialization due to the latest developments in the technology that promises to overcome the inherent bottleneck of high-temperature fuel cells, i.e., durability. According to the US Department of Energy (DOE), the stationary power generation system should have a lifetime of 40,000 h continuous operation. The efficiency of SOFCs is mainly dependent on their components such as anode, cathode, interconnect, and electrolyte. There are numerous factors affecting the efficiency of SOFCs that include the composition of the fuel, kinetics, and thermodynamics of the cell, and working temperature. In this paper, we have presented a comprehensive review of the recent developments to produce durable SOFCs for commercial stationary power generation systems. The review summarizes several prominent degradation mechanisms involved in the SOFC components and methods to reduce the degradation process. In addition, the methods and techniques adopted for the degradation analysis are fully demonstrated, followed by a detailed durability diagnostic through in-situ and ex-situ durability testing. The review is complemented by a lucid presentation of future research challenges and the knowledge gaps coupled with potential recommendations to fill the gaps. The new engineering designs, the material development and the new knowledge presented in this study could provide useful guidance for the key stakeholders, policymakers and power generation entities to commercially implement the application of durable SOFCs for stationary power generation.

Web URL: https://www.sciencedirect.com/science/article/pii/S030626192301228X

44. Zhu, B., Fan, L., Mushtaq, N., Raza, R., Sajid, M., Wu, Y., ... & Yun, S. (2021). Semiconductor electrochemistry for clean energy conversion and storage. Electrochemical Energy Reviews, 1-36.

ABSTRACT:

Semiconductors and the associated methodologies applied to electrochemistry have recently grown as an emerging field in energy materials and technologies. For example, semiconductor membranes and heterostructure fuel cells are new technological trend, which differ from the traditional fuel cell electrochemistry principle employing three basic functional components: anode, electrolyte, and cathode. The electrolyte is key to the device performance by providing an ionic charge flow pathway between the anode and cathode while preventing electron passage. In contrast, semiconductors and derived heterostructures with electron (hole) conducting materials have demonstrated to be much better ionic conductors than the conventional ionic electrolytes. The energy band structure and alignment, band bending and built-in electric field are all important elements in this context to realize the necessary fuel cell functionalities. This review further extends to semiconductor-based electrochemical energy conversion and storage, describing their fundamentals and working principles, with the intention of advancing the understanding of the roles of semiconductors and energy bands in electrochemical devices for energy conversion and storage, as well as applications to meet emerging demands widely involved in energy applications, such as photocatalysis/water splitting devices, batteries and solar cells. This review provides new ideas and new solutions to problems beyond the conventional electrochemistry and presents new interdisciplinary approaches to develop clean energy conversion and storage technologies.

Web URL: https://link.springer.com/article/10.1007/s41918-021-00112-8

45. Farhan, M., Ali, A., Ali, Z., & Raza, R. (2023). The Exploration of Cerium Metal Ions Effect on LaSrTiO3–δ Ceramic Anode for Fuel Cell. Russian Journal of Physical Chemistry A, 97(11), 2592-2602.

ABSTRACT:

Perovskite based materials have become an attractive anode for fuel cell due to the significant conductivity, carbon resistivity and sulphur tolerance. Doping of Ce on B-site of the $La_{0.4}Sr_{0.6}Ce_xTi_{1-x}O$\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$_{{3-\delta }}$$\end{document} (x = 0.02, 0.04, 0.06, 0.08) with different dopant concentrations is prepared using sol-gel technique. The synthesized material is analyzed by numerous techniques. X-ray diffraction confirmed the cubic perovskite structure (JCPDS 01-079- 0183) with average crystallite size

of 35 nm. UV–Vis spectroscopy revealed the red shift in band gap (2.76 eV) compared to LaSrTiO\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$_{{3-\delta }}$$\end{document}. Scanning electron microscopy shows the homogeneity and porosity in the prepared material. The observed particle size is in the range of 50–60 nm. The presence of the lanthanum, strontium, cerium, titanium and oxygen ions is confirmed by EDX. The Raman spectra and XRD, confirmed that cerium ions have been diffused in the lattice structure of LSTO\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$_{{3-\delta }}$$\end{document}. The $La_{0.4}Sr_{0.6}Ce_{0.08}Ti_{0.92}O$\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$_{{3-\delta }}$$\end{document} anode showed the highest conductivity of 2.67 S cm^{-1} with lower activation energy of 0.20 eV as compared to other three samples. The power density of 58 mW cm^{-2} at 600°C with 0.9 V OCV is achieved for the composition $La_{0.4}Sr_{0.6}Ce_{0.08}Ti_{0.92}O$\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$_{{3-\delta }}$$\end{document} using sub-bituminous fuel. The observed results show that prepared material is potential ceramic anode for direct carbon fuel cell.

Web URL: https://link.springer.com/article/10.1134/S0036024423110249

46. Lu, Y., Mushtaq, N., Shah, M. Y., Almutairi, B. S., Dong, Y., Yousaf, M., & Raza, R. (2023). Theoretical and experimental design for promoting the oxygen reduction activity of SrCoO3 perovskite-based cathode for PCFCs by bimetal-ions doping. International Journal of Hydrogen Energy, 48(87), 34034-34044.

ABSTRACT:

Low temperatures ceramic fuel cells (LT-CFCs) including solid oxide and proton conducting fuel cells (SOFCs/PCFCs), hold a great promise for abundant large-and small scaled real-application. Sluggish oxygen reduction reaction (ORR) activity at lower operating temperatures hindered the development of LT-CFCs. Strontium cobalt-based perovskite-oxides (SrCoO3−δ) materials have been frequently considered as a promising next-generation cathode for CFCs. Different doping stratigy are used to improve the mixed ionic (H^+/O^{2-}) and electronic conductivity of SrCoO3−δ, which help to extend the electrochemical reaction zone for oxygen reduction. Herein, we introduced bi-metal doping of La and Ce at B-site of SrCoO3−δ to produce

$SrCo_{0.8}Ce_{0.1}La_{0.1}O_{3-\delta}$ (SCCL) pervoskite structure for PCFCs cathode. The developed SLCC cathode exhibits ultra-low-area-specific polarization resistance of 0.11 $\Omega \cdot cm^2$ and large oxygen reduction reaction (ORR) response at intermediate operating temperatures. We have demonstrated power density of 510 $mWcm^{-2}$ using SLCC cathode over proton conducting $BaCe_{0.7}Zr_{0.2}Y_{0.1}O_{3-\delta}$ electrolyte at 600 °C and even with possible operation at 450 °C. The ORR activity of SLCC perovskites is found to strongly rely on the two proposed descriptors, where La and Ce doping at Co-site-in SrCoO3−δ located in the auspicious zone for predicting the moderate value of vacancy formation energy and ions migration barrier. The obtained results can further help to develop more functional SrCoO3−δ-based electro-catalysts for LT-CFCs and other related applications.

Web URL: https://www.sciencedirect.com/science/article/pii/S0360319923023728

47. Tariq, M. A., Ali, A., Nawaz, M. I., Hamid, A., Atif, M., & Raza, R. (2023). Experimental and Theoretical Study of Gallium–Doped Cerium Electrolyte for Fuel Cells. ACS Applied Energy Materials, 6(21), 10817-10828.

ABSTRACT:

Fuel cells produce clean and green power in an environmentally friendly way. An energy device fuel cell is used because of its higher efficiency and fuel flexibility. A number of efforts have been made to commercialize this technology by reducing its cost and operating temperature, and enhancing the durability. The operating temperature and performance of the cell depend on the electrolyte's stability and durability. Therefore, Ga–doped ceria electrolyte was synthesized by the coprecipitation technique. X–ray powder diffraction (XRD) spectra confirm the successful doping of gallium into ceria and reveal a cubic structure with crystallite size ranging from 50 to 60 nm. Scanning electron microscope (SEM) analysis confirmed the homogeneous surface morphology of the prepared material. The optical band gap shows a red shift compared to ceria. Thermal analysis shows that sample "d" has the lowest weight loss of 0.33% in the range 20–900 °C. It has been observed that the composition $Ga_{0.04}Ce_{0.96}O_{2-\delta}$ exhibited a maximum conductivity of 0.054 S cm^{-1} at 600 °C. The cell showed a power density of 86 mW cm^{-2} at 600 °C with an OCV of 1.02 V. Density functional theory depicts that gallium doping reduces the band gap and shifts the O 2p states toward Fermi level, due to which conductivity of the doped system is improved. The results reveal that Ga–doped ceria is an efficient electrolyte for fuel cells.

Web URL: https://pubs.acs.org/doi/full/10.1021/acsaem.3c01433

48. Li, J., Mushtaq, N., Shah, M. Y., Almutairi, B. S., Rauf, S., Raza, R., ... & Lu, Y. (2023). Large oxygen reduction response of CaFe2O4-WO3 heterostructure composite for protonic ceramic fuel cell cathode. Ceramics International, 49(18), 29736-29746.

ABSTRACT:

Protonic Ceramic fuel cells (PCFCs) hold great promise for many applications; however, their high operating temperature hinders their commercial use in practice. The crucial issue that limits the electrochemical performance of PCFCs (including oxygen and proton-ion-conducting) is the sluggish oxygen redox reaction (ORR) at the cathode surface at low operating temperatures. Herein, we have developed a C**aFe_2O_4-WO_3** heterostructure composite by interface-vacancy engineered for an efficient ORR electrocatalyst for LT-PCFCs. The C**aFe_2O_4-WO_3** heterostructure composite exhibits very low cathodic area-specific resistance (ASR) and high oxygen reduction reaction (ORR) activity response at low operating temperatures of 400–550 °C using a $BaCe_{0.7}Zr_{0.2}Y_{0.1}O_{3-\delta}$ (proton-conducting) electrolyte. We have demonstrated high-power density of 585 ± 2% mW-cm^{-2} with a current density of 1660 mA-cm^{-2} at 550 °C with H_2 fuel and atmospheric air as oxidant and even with possible operation at 400 °C. Moreover, the **$CaFe_2O_4$-WO_3 heterostructure composite** shows a very low proton migration energy and activation energy compared to individual $CaFe_2O_4$ and WO_3, helping to promote ORR activity. Various spectroscopic measurements, such as X-ray diffraction, high resolution transmission electron microscopy (HR-TEM), U-visible spectroscopy (UV–visible), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations are employed to understand the interfacial properties for the improved ORR electrocatalytic activity of the $CaFe_2O_4$-WO_3 heterostructure composite cathode. **Our obtained experimental and theoretical results can** further help to develop functional cobalt-free electrocatalysts for LT-PCFCs.

Web URL: https://www.sciencedirect.com/science/article/pii/S0272884223018023

49. Bukhari, M., Mohsin, M., Kayani, Z. N., Rasool, S., & Raza, R. (2023). The La+ 3-, Nd+ 3-, Bi+ 3-Doped Ceria as Mixed Conductor Materials for Conventional and Single-Component Solid Oxide Fuel Cells. Energies, 16(14), 5308.

ABSTRACT:

Clean energy devices are essential in today's environment to combat climate change and work towards sustainable development. In this paper, the potential materials $A_2Ce_2O_{7-\delta}$ (A = La^{+3}, Nd^{+3}, Bi^{+3}) were analyzed for clean energy devices, specifically for conventional and single-component solid oxide fuel cells (SC-SOFCs). The wet chemical route has been followed for the preparation of samples. X-ray diffraction patterns showed that all three samples exhibited a defected fluorite cubic structure. It also revealed the presence of dopants in the ceria, which was confirmed by the fingerprint region of FTIR. The optical behavior, fuel cell performance and electrochemical behavior were studied by UV–vis, fuel cell testing apparatus and EIS, respectively. The SEM results showed that all samples had irregular polygons. In Raman spectra, the F_{2g} mode corresponding to the space group (Fm3m) confirms the fluorite structure. The Raman spectra showed that $A_2Ce_2O_{7-\delta}$ (A = La^{+3}, Nd^{+3}, Bi^{+3}) have different trends. The conventional fuel cell performance showed that the maximum power density of $Bi_2Ce_2O_7$ was 0.65 Wcm^{-2} at 600 °C. The performance of $A_2Ce_2O_{7-\delta}$ (A = La^{3+}, Nd^{3+}, Bi^{3+}) as a single-

component fuel cell revealed that $Nd_2Ce_2O_{7-\delta}$ is the best choice with semiconductors conductors ZnO and NCAL. The highest power density (Pmax) of the $Nd_2Ce_2O_7$/ZnO was 0.58 Wcm^{-2}, while the maximum power output (Pmax) of the $Nd_2Ce_2O_7$/NCAL was 0.348 Wcm^{-2} at 650 °C. All the samples showed good agreement with the ZnO as compared to NCAL for SC-SOFCs.

Web URL: https://www.mdpi.com/1996-1073/16/14/5308

DEPARTMENT OF STATISTICS

1. Abbas, S., Farooq, M., Darwish, J. A., Shahbaz, S. H., & Shahbaz, M. Q. (2023). Truncated Weibull–exponential distribution: Methods and applications. Scientific Reports, 13(1), 20849.

ABSTRACT:

This paper introduces a truncated Weibull-exponential distribution and provides a thorough insight into its mathematical characteristics. These characteristics include moments, generating functions, inverse distribution function, and entropy. Various measures are also discussed about the distribution's reliability. A simulation study is carried out to assess the stability and consistency of the maximum likelihood estimates of the parameters. Finally, two social sciences data sets are used to assess the distribution's relevance in modeling real-world situations.

Web URL: https://www.nature.com/articles/s41598-023-48288-x

2. Gul, A., Sandhu, A. J., Farooq, M., Adil, M., Hassan, Y., & Khan, F. (2023). Half logistic-truncated exponential distribution: Characteristics and applications. Plos one, 18(11), e0285992.

ABSTRACT:

Gul and Mohsin 2021 developed a new modified form of renowned “Half logistic” distribution introduced by Balakrishnan (1991) and named it half logistic-truncated exponential distribution (HL-TEXPD). Some mathematical characteristics are studied, including hazard function, P^{th} percentile, moment generating function and Shannon entropy. Simulation study is performed to examine the behaviour of parameter estimates. The proposed model is fitted on three real data sets to check its efficacy. Additionally, TTT (total time on test) plot is drawn to study the failure rate of the three data sets. The results verdict that HL-TEXPD can be efficiently utilized in the field of engineering and medical sciences based on the data sets under study contrary to the classical and baseline models.

Web URL: https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0285992

3. Farooq, M., Gul, A., Alshanbari, H. M., & Khosa, S. K. (2023). Modeling of System Availability and Bayesian Analysis of Bivariate Distribution. Symmetry, 15(9), 1698.

ABSTRACT:

To meet the desired standard, it is important to monitor and analyze different engineering processes to obtain the desired output. The bivariate distributions have received a significant amount of attention in recent years due to their ability to describe randomness of natural as well as artificial mechanisms. In this article, a bivariate model is constructed by compounding two independent asymmetric univariate distributions and by using the nesting approach to study the effect of each component on reliability for better understanding. Furthermore, the Bayes analysis of system availability is studied by considering prior parametric variations in the failure time and repair time distributions. Basic statistical characteristics of marginal distribution like mean median and quantile function are discussed. We used inverse Gamma prior to study its frequentist properties by conducting a Monte Carlo Markov Chain (MCMC) sampling scheme.

Web URL: https://www.mdpi.com/2073-8994/15/9/1698

4. HASSAN, Y., FAROOQ, M., YASIR, S., & MURRAY, W. (2023). On Some New Exponential Ratio Estimator of Population Mean in Two Phase Sampling. Sains Malaysiana, 52(7), 2149-2162.

ABSTRACT:

In this paper, we suggest employing the exponential ratio estimator to estimate the mean of the study variable using a two-phase sample strategy with two modified auxiliary variables. Several researchers discussed the properties of the estimators they proposed and discovered that the estimators in their studies were relatively efficient. The estimators previously studied are listed chronologically in the appendix to this paper. In two phase sampling, the estimator's mean square errors and relative efficiencies are calculated using auxiliary variable information. To assess the properties of our proposed estimator, we noticed that it has a lower mean square error (MSE) than the classical ratio estimator and some other exponential ratio estimators. The estimator is more useful than other estimators in solving real-world issues, notably in engineering, environmental science, management, and biological sciences. The proposed estimator has been applied to real-world data sets such as BRICS, Son's Head Measurement, Number of Hospital Beds, Sale Price of Residence, Ambient Pressure (AP), and Heating Load. In survey research, our suggested estimator has also been demonstrated to be more effective

Web URL: https://journalarticle.ukm.my/22601/1/STT%2020.pdf

5. Iqbal, J., Noor-ul-Amin, M., Khan, I., AlQahtani, S. A., Yasmeen, U., & Ahmad, B. (2023). A novel Bayesian Max-EWMA control chart for jointly monitoring the process mean and variance: an application to hard bake process. Scientific Reports, 13(1), 21224.

ABSTRACT:

In this article, we introduce a novel Bayesian Max-EWMA control chart under various loss functions to concurrently monitor the mean and variance of a normally distributed process. The Bayesian Max-EWMA control chart exhibit strong overall performance in detecting shifts in both mean and dispersion across various magnitudes. To evaluate the performance of the proposed control chart, we employ Monte Carlo simulation methods to compute their run length characteristics. We conduct an extensive comparative analysis, contrasting the run length performance of our proposed charts with that of existing ones. Our findings highlight the heightened sensitivity of Bayesian Max-EWMA control chart to shifts of diverse magnitudes. Finally, to illustrate the efficacy of our Bayesian Max-EWMA control chart using various loss functions, we present a practical case study involving the hard-bake process in semiconductor manufacturing. Our results underscore the superior performance of the Bayesian Max-EWMA control chart in detecting out-of-control signals.

Web URL: https://nature.com/articles/s41598-023-48532-4

6. Khan, I., Noor-ul-Amin, M., Khan, D. M., Ismail, E. A., Yasmeen, U., & Rahimi, J. (2023). Monitoring the process mean under the Bayesian approach with application to hard bake process. Scientific Reports, 13(1), 20723.

ABSTRACT:

This study introduces the Bayesian adaptive exponentially weighted moving average (AEWMA) control chart within the framework of measurement error, examining two separate loss functions: the squared error loss function and the linex loss function. We conduct an analysis of the posterior and posterior predictive distributions utilizing a conjugate prior. In the presence of measurement error (ME), we employ a linear covariate model to assess the control chart's effectiveness. Additionally, we explore the impacts of measurement error by investigating multiple measurements and a method involving linearly increasing variance. We conduct a Monte Carlo simulation study to assess the control chart's performance under ME, examining its run length profile. Subsequently, we offer a specific numerical instance related to the hard-bake process in semiconductor manufacturing, serving to verify the functionality and practical application of the suggested Bayesian AEWMA control chart when confronted with ME.

Web URL: https://www.nature.com/articles/s41598-023-48206-1

7. Khan, I., Noor-ul-Amin, M., Muhammad Khan, D., Khalil, U., Ismail, E. A., Yasmeen, U., & Ahmad, B. (2023). Bayesian AEWMA control chart under ranked set sampling with application to reliability engineering. Scientific Reports, 13(1), 20020.

ABSTRACT:

The article introduces a novel Bayesian AEWMA Control Chart that integrates different loss functions (LFs) like the square error loss function and Linex loss function under an informative prior for posterior and posterior predictive distributions, implemented across diverse ranked set sampling (RSS) designs. The main objective is to detect small to moderate shifts in the process mean, with the average run length and standard deviation of run length serving as performance measures. The study employs a hard bake process in semiconductor production to demonstrate the effectiveness of the proposed chart, comparing it with existing control charts through Monte Carlo simulations. The results underscore the superiority of the proposed approach, particularly under RSS designs compared to simple random sampling (SRS), in identifying out-of-control signals. Overall, this study contributes a comprehensive method integrating various LFs and RSS schemes, offering a more precise and efficient approach for detecting shifts in the process mean. Real-world applications highlight the heightened sensitivity of the suggested chart in identifying out-of-control signals compared to existing Bayesian charts using SRS.

Web URL: https://www.nature.com/articles/s41598-023-47324-0

8. Sarwar, M. A., Noor-ul-Amin, M., Khan, I., Ismail, E. A., Sumelka, W., & Nabi, M. (2023). A Weibull process monitoring with AEWMA control chart: an application to breaking strength of the fibrous composite. *Scientific Reports*, *13*(1), 19873.

ABSTRACT:

In recent times, there has been a growing focus among researchers on memory-based control charts. The Exponentially Weighted Moving Average (EWMA) and Cumulative Sum (CUSUM) charts and the adaptive control charting approaches got the attention. Control charts are commonly employed to oversee processes, assuming the monitored variable follows a normal distribution. However, it's worth noting that this assumption does not hold true in many real-world situations. The use of the algebraic expression for normalization, which can be used for all kinds of skewed distributions with a closed-form distribution function, using the proposed continuous function to adapt a smoothing constant, motivates this study. In the present manuscript, we design an EWMA statistic-based adaptive control chart to monitor the irregular variations in the mean of two parametric Weibull distribution and use Hasting approximation for normalization. The adaptive control charts are used to update the smoothing constant according to the estimated shift. Here we use the proposed continuous function to adapt the smoothing constant. The average run length and standard deviation of run length are calculated under different parameter settings. The effectiveness of the proposed chart is argued in terms of ARLs over the considered EWMA chart through Monte-Carlo (MC) simulation method. The proposed chart is examined, followed by a real data set to demonstrate the design and application procedures.

Web URL: https://www.nature.com/articles/s41598-023-47159-9

9. Noor-ul-Amin, M., & Atif Sarwar, M. (2023). Design of a new adaptive MEWMA chart to monitor the mean. Journal of Statistical Computation and Simulation, 93(16), 2888-2905.

ABSTRACT:

The adaptive MEWMA (AMEWMA) charts have been broadly perceived as an effective process monitoring instrument due to the efficient detection of the mean shifts of diverse sizes. This study proposes an AMEWMA control chart to observe the irregular variations in the mean vector of the process which follows the multivariate normal distribution. The idea is to assess the mean shift by using an unbiased estimator and after that adapt the smoothing constant of plotting EWMA statistic through a continuous function. As an evaluation tool, the run-length profiles are computed by using the Monte Carlo simulation method. The proposed AMEWMA chart is proved to be efficient in shift detection as compared to the MEWMA and existing AMEWMA charts. The application of the proposed chart is shown by utilizing a real-life dataset from a case study of process capability for turning aluminum pins where six quality characteristics are to be observed

Web URL: https://www.tandfonline.com/doi/full/10.1080/00949655.2023.2213372

10. Khan, I., Noor-ul-Amin, M., Khan, D. M., Ismail, E. A., & Sumelka, W. (2023). Monitoring of manufacturing process using bayesian EWMA control chart under ranked based sampling designs. Scientific Reports, 13(1), 18240.

ABSTRACT:

Control charts, including exponentially moving average (EWMA) , are valuable for efficiently detecting small to moderate shifts. This study introduces a Bayesian EWMA control chart that employs ranked set sampling (RSS) with known prior information and two distinct loss functions (LFs), the Square Error Loss function (SELF) and the Linex Loss function (LLF), for posterior and posterior predictive distributions. The chart's performance is assessed using average run length (ARL) and standard deviation of run length (SDRL) profiles, and it is compared to the Bayesian EWMA control chart based on simple random sampling (SRS). The results indicate that the proposed control chart detects small to moderate shifts more effectively. The application in semiconductor manufacturing provides concrete evidence that the Bayesian EWMA control chart, when implemented with RSS schemes, demonstrates a higher degree of sensitivity in detecting deviations from normal process behavior. Comparison to the Bayesian EWMA control chart using SRS, it exhibits a superior ability to identify and flag instances where the manufacturing process is going out of control. This heightened sensitivity is critical for promptly addressing and rectifying issues, which ultimately contributes to improved quality control in semiconductor production.

Web URL: https://www.nature.com/articles/s41598-023-45553-x

11. Noor-ul-Amin, M., Sarwar, M. A., Emam, W., Tashkandy, Y., Yasmeen, U., & Nabi, M. (2023). Adaptive multivariate dispersion control chart with application to bimetal thermostat data. Scientific Reports, 13(1), 18137.

ABSTRACT:

Adaptive EWMA (AEWMA) control charts have gained remarkable recognition by monitoring productions over a wide range of shifts. The adaptation of computational statistic as per system shift is the main aspect behind the proficiency of these charts. In this paper, a function-based AEWMA multivariate control chart is suggested to monitor the stability of the variance–covariance matrix for normally distributed process control. Our approach involves utilizing an unbiased estimator applying the EWMA statistic to estimate the process shift in real-time and adapt the smoothing or weighting constant using a suggested continuous function. Preferably, the Monte Carlo simulation method is utilized to determine the characteristics of the suggested AEWMA chart in terms of proficient detection of process shifts. The underlying computed results are compared with existing EWMA and existing AEWMA charts and proved to outperform in providing quick detection for different sizes of shifts. To illustrate its real-life application, the authors employed the concept in the bimetal thermostat industry dataset. The proposed research contributes to statistical process control and provides a practical tool for the solution while monitoring covariance matrix changes.

Web URL: https://www.nature.com/articles/s41598-023-45399-3

12. Riaz, A., Noor-ul-Amin, M., Emam, W., Tashkandy, Y., Yasmeen, U., & Rahimi, J. (2023). Adaptive EWMA control chart for monitoring the coefficient of variation under ranked set sampling schemes. Scientific Reports, 13(1), 17617.

ABSTRACT:

In this study, we introduce an Adaptive Exponentially Weighted Moving based Coefficient of Variation (AEWMCV) control chart, designed to address situations where the process mean fluctuates over time and the standard deviation of the process changes linearly with the process mean. To enhance the efficiency and effectiveness of the control chart, we integrate the ranked set sampling method and its modified schemes, such as Simple Random Sampling, Quartile RSS, Median RSS, and Extreme RSS. The performance of the proposed AEWMCV control chart and the studied CV control charts are evaluated using the Average Run Length and Standard Deviation of Run Length metrics. Our findings reveal that the proposed control chart outperforms the existing CV control charts, especially in detecting slight to moderate changes in the process CV. To illustrate the practical applicability of the suggested control chart, we present an example demonstrating its use on a real dataset. The results highlight the superior performance of the AEWMCV control chart in accurately detecting and responding to changes in the process CV. In conclusion, our study introduces an innovative AEWMCV control chart that combines ranked set sampling and its modified schemes to enhance performance in scenarios

with fluctuating process means and changing standard deviations. The proposed control chart proves to be more effective in detecting subtle variations in the process CV compared to traditional CV control charts. This research provides a valuable contribution to the field of control chart methodology, especially when dealing with challenging or costly data collection scenarios.

Web URL: https://www.nature.com/articles/s41598-023-45070-x

13. Noor-ul-Amin, M., & Arshad, A. (2023). Homogeneously weighted moving average-variance control chart using auxiliary information. Communications in Statistics-Simulation and Computation, 52(10), 4891-4908.

ABSTRACT:

In this study, a variance control chart is proposed with some modifications in terms of the rapid detection of process shifts by using the homogenously weighted moving average (HWMAHWMA) statistic by using the information from an auxiliary variable. The proposed HWMAHWMA chart is a new memory type variance control chart with a three-parameter log transformation that operates by assigning the specified weights to the most recent value. All previous samples are allotted with an equal proportion of the remaining smoothing parameter weight. The remaining weights put their effect as a counterpart within the smoothing parameter and the current observations take the maximum of it. To study the performance of the proposed chart the respective run length properties are determined by Monte Carlo simulations and extensively presented in the tables. The comparison has been made with the existing exponentially weighted moving average (EWMAEWMA) variance control chart. It is figured out that the proposed control chart is sensitive to process shift by using the auxiliary information with a high degree of correlation. The real-life dataset is selected from an industrial production environment to demonstrate the implementation of the proposed chart.

Web URL: https://www.tandfonline.com/doi/full/10.1080/03610918.2021.1974039#abstract

14. Zahid, R., Noor-ul-Amin, M., Khan, I., AlQahtani, S. A., Pathak, P. K., & Rahimi, J. (2023). Combination of memory type ratio and product estimators under extended EWMA statistic with application to wheat production. Scientific Reports, 13(1), 13547.

ABSTRACT:

The extended exponential weighted moving average (EEWMA) statistic is a memory type statistic that uses past observations along with the current information for the estimation of a population parameter to improve the efficiency of the estimators. This study utilized the EEWMA statistic to estimate the population mean with a suitable auxiliary variable. The ratio and product estimators are proposed for the surveys that are time-based by using current information along with that information. The approximate mean square errors are computed for

the proposed memory type estimators and mathematical comparison is discussed to demonstrate the efficiency of the estimator. The simulation study was carried out to evaluate the performance of the proposed memory type estimators. It can be seen from the results that the efficiency of the estimator enhances by utilizing the current sample as well as past information. A real-life example is presented to illustrate the usage of proposed estimators.

Web URL: https://www.nature.com/articles/s41598-023-40687-4

15. Noor-ul-Amin, M., Aslam, I., & Feroze, N. (2023). Joint monitoring of mean and variance using Max-EWMA for Weibull process. Communications in Statistics-Simulation and Computation, 52(7), 3257-3272.

ABSTRACT:

Simultaneously monitoring of process mean and dispersion for the normal process has gained considerable attention. In this manuscript, we have proposed a maximum exponentially weighted moving average (*Max-EWMA*) control chart for joint monitoring of mean and dispersion using the inverse response function when the process follows Weibull distribution. The average run length (*ARL*) and the standard deviation of run length (*SDRL*) are used as the evaluation tools. The proposed control chart is compared with the available *Max-EWMA* control chart. We conclude that the proposed control chart is more sensitive than the considered control chart. The application of the proposed control chart is presented with the aid of two examples.

Web URL: https://www.tandfonline.com/doi/full/10.1080/03610918.2021.1931322#abstract

16. Abeysingha, N., Abeysundara, H., Akhter, A. S., Alawatugoda, J., Amarakeerthi, S., Amarasekara, M. G. T. S., ... & Galhena, G. (2023). List of Referees-Volume 51 (2023). of the National Science Foundation, 719.

ABSTRACT:

In real life, the distribution of the errors during any life testing of products or process does not meet the assumption of normality. Statistical process control (SPC) is defined as the use of statistical techniques to control a process or production method. SPC tools and procedures can help to monitor process behaviour, discover problems in internal systems, and find solutions for production issues. To identify and remove the variation in different reliability processes and to monitor the reliability of machines where the number of errors follows skewed distributions, we develop control charts to keep the process in control. For such situations, we have modified the existing control charts such as Shewhart control chart, exponentially weighted moving average (EWMA), hybrid exponentially weighted moving average (HEWMA) and extended exponentially weighted moving average (EEWMA) control charts. The current study introduced classical estimator based modified control charts for phase-II monitoring by assuming that the errors occur during the process follow skewed distribution called Beta Lehmann 2 Power

function distribution (BL2PFD). The proposal for these control charts is based on the percentile estimator. We have compared all these control charts using Monte Carlo simulation studies and real-life applications to compare the proposed control charts. This study shows that an EEWMA control chart based on PE performs better than Shewhart, EWMA and HEWMA control charts, when the underlying distribution of the errors in process monitoring follows BL2PFD. These findings can be useful for researchers and practitioners in dealing with production errors and optimizing the output.

Web URL: http://www.nsf.ac.lk/images/nsf/jnsf/JNSF_Volume_51_No_3.pdf#page=97

17. Zaka, A., Jabeen, R., Ahmad, M., Aljohani, H. M., & Helmi, M. M. (2024). Control theory for skewed distribution under operation side of the telecommunication industry and hard-bake process in the semiconductor manufacturing process. Measurement and Control, 57(6), 703-723.

ABSTRACT:

Statistical process control basically involves inspecting a random sample of the output from a process and deciding whether the process is producing products with characteristics that fall within a predetermined range. It is used extensively in the field of reliability engineering. The reliability of the production process is thoroughly monitored for any internal variation using the SPC. The aim is always to settle such variations through a proper control monitoring. If the underlying distribution of the process is known to the researcher than the use of parametric control charts are useful but in many cases when there is doubt about the distribution of the process then it is preferred to use non parametric control charts. In this paper we propose the modified Exponentially weighted moving average (EWMA), Double Exponentially weighted moving average (DEWMA), Hybrid Exponentially weighted moving average (HEWMA), Extended Exponentially weighted moving average (EEWMA), Modified Exponentially weighted moving average (MEWMA) and mix- type control charts by mixing these control charts with Tukey control chart EWMA-TCC, DEWMA-TCC, HEWMA-TCC, EEWMA-TCC, MEWMA-TCC for the shape parameter of the Kumaraswamy Lehmann-2 Power function distribution (KL2PFD).

Web URL: https://journals.sagepub.com/doi/full/10.1177/00202940231214842

18. Chaudhary, A. M., Sanaullah, A., Hanif, M., Almazah, M. M., Albasheir, N. A., & Al-Duais, F. S. (2023). Efficient monitoring of a parameter of non-normal process using a robust efficient control chart: a comparative study. Mathematics, 11(19), 4157.

ABSTRACT:

The control chart is a fundamental tool in statistical process control (SPC), widely employed in manufacturing and construction industries for process monitoring with the primary objective of

maintaining quality standards and improving operational efficiency. Control charts play a crucial role in identifying special cause variations and guiding the process back to statistical control. While Shewhart control charts excel at detecting significant shifts, EWMA and CUSUM charts are better suited for detecting smaller to moderate shifts. However, the effectiveness of all these control charts is compromised when the underlying distribution deviates from normality. In response to this challenge, this study introduces a robust mixed EWMA-CUSUM control chart tailored for monitoring processes characterized via symmetric but non-normal distributions. The key innovation of the proposed approach lies in the integration of a robust estimator, based on order statistics, that leverages the generalized least square (GLS) technique developed by Lloyd. This integration enhances the chart's robustness and minimizes estimator variance, even in the presence of non-normality. To demonstrate the effectiveness of the proposed control chart, a comprehensive comparison is conducted with several well-known control charts. Results of the study clearly show that the proposed chart exhibits superior sensitivity to small and moderate shifts in process parameters when compared to its predecessors. Through a compelling illustrative example, a real-life application of the enhanced performance of the proposed control chart is provided in comparison to existing alternatives.

Web URL: https://www.mdpi.com/2227-7390/11/19/4157

19. Saleem, I., Sanaullah, A., Al-Essa, L. A., Bashir, S., & Al Mutairi, A. (2023). Efficient estimation of population variance of a sensitive variable using a new scrambling response model. Scientific Reports, 13(1), 19913.

ABSTRACT:

This study introduces a pioneering scrambling response model tailored for handling sensitive variables. Subsequently, a generalized estimator for variance estimation, relying on two auxiliary information sources, is developed following this novel model. Analytical expressions for bias, mean square error, and minimum mean square error are meticulously derived up to the first order of approximation, shedding light on the estimator's statistical performance. Comprehensive simulation experiments and empirical analysis unveil compelling results. The proposed generalized estimator, operating under both scrambling response models, consistently exhibits minimal mean square error, surpassing existing estimation techniques. Furthermore, this study evaluates the level of privacy protection afforded to respondents using this model, employing a robust framework of simulations and empirical studies.

Web URL: https://www.nature.com/articles/s41598-023-45427-2

20. Maqsood, M., Sanaullah, A., Mahmood, Y., Al-Rezami, A. Y., & Abdalla, M. Z. (2023). Efficient control chart-based monitoring of scale parameter for a process with heavy-tailed non-normal distribution. AIMS Mathematics, 8(12), 30075-30101.

ABSTRACT:

Statistical process control is a procedure of quality control that is widely used in industrial processes to enable monitoring by using statistical techniques. All production processes are faced with natural and unnatural variations. To maintain the stability of the production process and reduce variation, different tools are used. Control charts are significant tools to monitor a production process. In this article, we design an extended exponentially weighted moving average (EEWMA) chart under the assumption of inverse Maxwell (IM) distribution, an IM EEWMA (IMEEWMA) control chart. We have estimated the performance of the proposed chart in terms of various run-length (RL) properties, including the average RL, standard deviation of the RL and median RL. We have also carried out a comparative analysis of the proposed chart with the existing Shewhart-type chart for IM distribution (VIM chart) and IM exponential weighted moving average (IMEWMA) chart. We observed that the proposed IMEEWMA chart performed better than the VIM chart and IMEWMA chart in terms of the ability to detect small and moderate shifts. To demonstrate its practical application, we have applied the IMEEWMA chart, along with existing control charts, to monitor the lifetime of car brake pad data. This real-world example illustrates the superiority of the IMEEWMA chart over its counterparts in industrial scenarios.

Web URL: https://www.aimspress.com/aimspress-data/math/2023/12/PDF/math-08-12-1538.pdf

21. Ahmed, A., Sanaullah, A., Oral, E., & Hanif, M. (2023). Robust ratio estimators of population mean for skewed and contaminated population. Journal of Statistical Computation and Simulation, 93(5), 800-817.

ABSTRACT:

The efficiency of the traditional ratio estimator decreases with the presence of outliers, inliers or when the underlying distribution is not normal. To improve the efficiency, we propose new robust ratio estimators utilizing the Lloyd's robust estimator and modified maximum likelihood estimator (MMLE), and provide their theoretical properties. We calculate the mean square error and relative efficiency of the proposed estimators and compare its performance with some other existing traditional estimators via a simulation study under various contamination or misspecification models. Further, we evaluate the exact value of the mean square error and to compare the performance of the proposed estimators using the numerical illustrations.

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