

Research Publications in Year 2023

Sr. No	Reference
1.	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. <i>Computational and Theoretical Chemistry</i> , 1220, 113990.
2.	Sajid, H., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Donor- π -Acceptor N-Methyl-4, 5-Diazacarbazole Based Ultra-High Performance Organic Solar Cells: A Density Functional Theory Study. <i>Energy Technology</i> , 11(1), 2201164.
3.	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. <i>Chemosphere</i> , 313, 137603.
4.	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. <i>Materials Science in Semiconductor Processing</i> , 160, 107468.
5.	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. <i>Chemical Physics</i> , 570, 111894.
6.	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. <i>Diamond and Related Materials</i> , 135, 109826.
7.	Ahmed, K., Bashir, M., Bano, R., Sarfraz, M., Khan, H. U., Khan, S., ... & Arshad, M. (2023). Potent heteroaromatic hydrazone based 1, 2, 4-triazine motifs: synthesis, anti-oxidant activity, cholinesterase inhibition, quantum chemical and molecular docking studies. <i>Journal of Molecular Structure</i> , 1284, 135383.
8.	Kosar, N., Zari, L., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Giant NLO response and ultraviolet transparency of superalkalis decorated C6O6Li6 complexes; a DFT perspective. <i>Physica Scripta</i> , 98(6), 065909.
9.	Asif, M., Sajid, H., Ayub, K., Gilani, M. A., Anwar, N., & Mahmood, T. (2023). Therapeutic potential of oxo-triarylmethyl (oxTAM) as a targeted drug delivery system for nitrosourea and fluorouracil anticancer drugs; A first principles insight. <i>Journal of Molecular Graphics and Modelling</i> , 122, 108469.
10.	Allangawi, A., Jalal, K. A., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Chemical sensing ability of aminated graphdiyne (GDY-NH ₂) toward highly toxic organic volatile

	pollutants. <i>Computational and Theoretical Chemistry</i> , 1222, 114079.
11.	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. <i>International Journal of Hydrogen Energy</i> , 48(44), 16663-16677.
12.	Rafique, A., Muhammad, S., Iqbal, J., Al-Sehemi, A. G., Alshahrani, M. Y., Ayub, K., & Gilani, M. A. (2023). Exploring the inhibitory potential of novel piperidine-derivatives against main protease (Mpro) of SARS-CoV-2: A hybrid approach consisting of molecular docking, MD simulations and MMPBSA analysis. <i>Journal of molecular liquids</i> , 382, 121904.
13.	Rehman, F., Khan, A. J., Sama, Z. U., Alobaid, H. M., Gilani, M. A., Safi, S. Z., ... & 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. <i>Frontiers in Pharmacology</i> , 14, 1146562.
14.	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. <i>Fuel</i> , 350, 128840.
15.	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. <i>Physical Chemistry Chemical Physics</i> , 25(30), 20430-20450.
16.	Asif, M., Qureshi, S., Sajid, H., Kosar, N., Gilani, M. A., Ayub, K., ... & Mahmood, T. (2023). Sensing Performance of Heptazine-Based C3N4 Quantum Dot Toward Highly Toxic Environmental Pollutants, Amides, and Acetyl Derivatives. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 1-14.
17.	Yaqoob, J., Tabassum, S., AlMohamadi, H., Mahmood, T., Ayub, K., Khan, A. L., ... & Gilani, M. A. (2023). Exploring the second-order polarizability of copper doped silicon carbide nanocluster: toward a new NLO material. <i>Physica Scripta</i> , 98(9), 095516.
18.	Sohaib, M., Sajid, H., Sarfaraz, S., Hamid, M. H. S. A., Gilani, M. A., Ans, M., ... & Ayub, K. (2023). Enhanced nonlinear optical response of alkalides based on stacked Janus all-cis-1, 2, 3, 4, 5, 6-hexafluorocyclohexane. <i>Heliyon</i> , 9(9).
19.	Kosar, N., Wajid, S., Ayub, K., Gilani, M. A., Arfan, N. H. B. Z., Hamid, M. H. S. A., ... & Mahmood, T. (2023). Giant NLO response and deep ultraviolet transparency of dual (alkali/alkaline earth) metals doped C6O6Li6 electrides. <i>Heliyon</i> , 9(8).
20.	Sajid, H., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Donor- π -Acceptor N-Methyl-4, 5-Diazacarbazole Based Ultra-High Performance Organic Solar Cells: A Density Functional Theory Study. <i>Energy Technology</i> , 11(1), 2201164.
21.	Allangawi, A., Kosar, N., Ayub, K., Gilani, M. A., Zainal Arfan, N. H. B., Hamid, M. H. S. A., ... & Mahmood, T. (2023). Decorating Mg12O12 nanocage with late first-row transition metals to

	act as single-atom catalysts for the hydrogen evolution reaction. <i>ACS omega</i> , 8(41), 37820-37829.
22.	Rafique, A., Muhammad, S., Iqbal, J., Al-Sehemi, A. G., Alshahrani, M. Y., Ayub, K., & Gilani, M. A. (2023). Exploring the inhibitory potential of novel piperidine-derivatives against main protease (Mpro) of SARS-CoV-2: A hybrid approach consisting of molecular docking, MD simulations and MMPBSA analysis. <i>Journal of molecular liquids</i> , 382, 121904.
23.	Ahmed, K., Bashir, M., Bano, R., Sarfraz, M., Khan, H. U., Khan, S., ... & Arshad, M. (2023). Potent heteroaromatic hydrazone based 1, 2, 4-triazine motifs: synthesis, anti-oxidant activity, cholinesterase inhibition, quantum chemical and molecular docking studies. <i>Journal of Molecular Structure</i> , 1284, 135383.
24.	Yaqoob, J., Tabassum, S., Mahmood, T., Ayub, K., Khan, A. L., Yasin, M., ... & Gilani, M. A. (2023). A Rational Design of Alkali Metal-Doped Germanium Carbide Nanoclusters for High Nonlinear Optical Response and Ultraviolet Transparency. <i>JOM</i> , 75(12), 5893-5908.
25.	Rasul, R., Mahmood, T., Ayub, K., Joya, K. S., Anwar, F., Saari, N., ... & Gilani, M. A. (2023). Alkali metals doped cycloparaphenylene nano hoops: Promising nonlinear optical materials with enhanced performance. <i>Heliyon</i> , 9(11).
26.	Ullah, F., Gilani, M. A., Imran, M., Ayub, K., & Mahmood, T. (2023). Potential of first row transition metal decorated graphtriyne quantum dots as single atom catalysts towards hydrogen evolution reaction (HER). <i>Physica Scripta</i> , 98(11), 115308.
27.	Kosar, N., Kanwal, S., Hamid, M. H. S., Ayub, K., Gilani, M. A., Imran, M., ... & Mahmood, T. (2023). Role of Delocalization, Asymmetric Distribution of π -Electrons and Elongated Conjugation System for Enhancement of NLO Response of Open Form of Spiropyran-Based Thermochromes. <i>Molecules</i> , 28(17), 6283.
28.	Batool, M., Farooqui, S. R., Gilani, M. A., Tabassum, S., & Junaid, H. M. (2023). Effect of conjugation in 4-amino phenazone based Schiff bases on their chemosensing of F-and OH-ions- Experimental and DFT study.
29.	Aslam, A. A., Irshad, A., Nazir, M. S., & Atif, M. (2023). A review on covalent organic frameworks as adsorbents for organic pollutants. <i>Journal of Cleaner Production</i> , 136737.
30.	Mahboob, I., Shafiq, I., Shafique, S., Akhter, P., Munir, M., Saeed, M., ... & Hussain, M. (2023). Porous Ag ₃ VO ₄ /KIT-6 composite: Synthesis, characterization and enhanced photocatalytic performance for degradation of Congo Red. <i>Chemosphere</i> , 311, 137180.
31.	Aslam, A. A., Irshad, A., Nazir, M. S., & Atif, M. (2023). A review on covalent organic frameworks as adsorbents for organic pollutants. <i>Journal of Cleaner Production</i> , 136737.
32.	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. <i>Chemosphere</i> , 313, 137418.
33.	Akhter, P., Bhatti, T. Y., Shafiq, I., Jamil, F., Nazar, R., Nazir, M. S., ... & Park, Y. (2023). Antioxidant activity of sea buckthorn (<i>Hippophae rhamnoides</i>) seed oil extracted using various organic solvents. <i>Korean Journal of Chemical Engineering</i> , 40(12), 2914-2920.
34.	Rafiq, A., Aslam, S., Ahmad, M., Nazir, M. S., Farooq, A., & Sultan, S. (2023). Recent synthetic approaches towards thienothiophenes: a potential template for biologically active compounds. <i>Molecular diversity</i> , 1-29.
35.	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. <i>Polymer-Plastics Technology and Materials</i> , 62(6), 790-799.
36.	Aslam, A. A., Hassan, S. U., Saeed, M. H., Kokab, O., Ali, Z., Nazir, M. S., ... & Aslam, A. A. (2023). Cellulose-based adsorbent materials for water remediation: Harnessing their potential in heavy metal and dye removal. <i>Journal of Cleaner Production</i> , 138555.
37.	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 CeO ₂ nanoparticles for electrochemical detection of ethanol. <i>Microchimica Acta</i> , 190(5), 172.
38.	Akhtar, M. N., Makhdoom, S., Nazir, M. S., Yousaf, M., & Khan, M. A. (2023). Microstructural and magnetic properties of transition and rare-earth metals-substituted cobalt nanoferrites. In <i>Magnetic Nanoferrites and their Composites</i> (pp. 87-116). Woodhead Publishing.
39.	Iftikhar, 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. <i>Journal of Natural Fibers</i> , 20(1), 2145411.
40.	Abbas, A., Mansoor, S., Nawaz, M. H., Chaudhry, A. A., Ijaz, K., Riaz, S., & Hayat, A. (2023). Growth of diazonium-functionalized ZnO nanoflakes on flexible carbon cloth for electrochemical sensing of acetone in the liquid phase. <i>RSC advances</i> , 13(17), 11537-11545.
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42.	Hamza, M., Ahmad, A., Tariq, M., Riaz, S., & Rahim, A. (2023). Metal-organic frameworks (an overview). <i>Nanomaterial-Based Metal Organic Frameworks for Single Atom Catalysis</i> , 1-38.
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44.	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. <i>ACS Sustainable Chemistry & Engineering</i> , 11(11), 4299-4307.
45.	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. <i>JOM</i> , 76(2), 646-655.
46.	Akhter, P., Bhatti, T. Y., Shafiq, I., Jamil, F., Nazar, R., Nazir, M. S., & Park, Y. (2023). Antioxidant activity of sea buckthorn (<i>Hippophae rhamnoides</i>) seed oil extracted using various organic solvents. <i>Korean Journal of Chemical Engineering</i> , 40(12), 2914-2920.
47.	Muqaddas, S., Aslam, H., Hassan, S. U., Ashraf, A. R., Asghar, M. A., Ahmad, M., ... & Ali, A. (2023). Electrochemical sensing of glucose and ascorbic acid via POM-based CNTs fiber electrode. <i>Materials Science and Engineering: B</i> , 293, 116446.
48.	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. <i>Cellulose</i> , 30(12), 7519-7533.
49.	Siddiq, 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. <i>Micromachines</i> , 14(5), 899.
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