Department of Chemistry

COMSATS University Islamabad, Lahore Campus

Defence Road, Off Raiwind Road Lahore Ph: 042-111 001 007 (857)

Research Publications in Year 2023-2024

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. Computational and Theoretical Chemistry, 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. Energy Technology, 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. *Chemosphere*, *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. *Materials Science in Semiconductor Processing*, *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. *Chemical Physics*, *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. *Diamond and Related Materials*, *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. *Journal of Molecular Structure*, *1284*, 135383.
8.	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.
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. *Journal of Molecular Graphics and Modelling*, *122*, 108469.
10.	Allangawi, A., Jalal, K. A., Ayub, K., Gilani, M. A., & Mahmood, T. (2023). Chemical sensing ability of aminated graphdiyne (GDY-NH2) toward highly toxic organic volatile pollutants. *Computational and Theoretical Chemistry*, *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. *International Journal of Hydrogen Energy*, *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. *Journal of molecular liquids*, *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. *Frontiers in Pharmacology*, *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. *Fuel*, *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. *Physical Chemistry Chemical Physics*, *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. *Journal of Inorganic and Organometallic Polymers and Materials*, 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. *Physica Scripta*, *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. *Heliyon*, *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. *Heliyon*, *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. *Energy Technology*, *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. *ACS omega*, *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. *Journal of molecular liquids*, *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. *Journal of Molecular Structure*, *1284*, 135383.
24.	Yaqoob, J., Tabasssum, 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. *JOM*, *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 nanohoops: Promising nonlinear optical materials with enhanced performance. *Heliyon*, *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). *Physica Scripta*, *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. *Molecules*, *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. *Journal of Cleaner Production*, 136737.
30.	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.
31.	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*, 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. *Chemosphere*, *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 (Hippophae rhamnoides) seed oil extracted using various organic solvents. *Korean Journal of Chemical Engineering*, *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. *Molecular diversity*, 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. *Polymer-Plastics Technology and Materials*, *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. *Journal of Cleaner Production*, 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 CeO2 nanoparticles for electrochemical detection of ethanol. *Microchimica Acta*, *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 *Magnetic Nanoferrites and their Composites* (pp. 87-116). Woodhead Publishing.
39.	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.
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. *RSC advances*, *13*(17), 11537-11545.
41.	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.
42.	Hamza, M., Ahmad, A., Tariq, M., Riaz, S., & Rahim, A. (2023). Metal–organic frameworks (an overview). *Nanomaterial-Based Metal Organic Frameworks for Single Atom Catalysis*, 1-38.
43.	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.
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. *ACS Sustainable Chemistry & Engineering*, *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. *JOM*, *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 (Hippophae rhamnoides) seed oil extracted using various organic solvents. *Korean Journal of Chemical Engineering*, *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. *Materials Science and Engineering: B*, *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. *Cellulose*, *30*(12), 7519-7533.
49.	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.
50.	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.
51.	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.