

Curriculum Vitae



Dr. MUHAMMAD YAR (Assistant Professor Chemistry)

Department of Physiology and Biochemistry, Cholistan University of Veterinary and Animal Sciences Bahawalpur, 63100 (Pakistan).

PERSONAL DATA

Father's Name: Manzoor Hussain

Date of Birth : 1st January 1983

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Main Scientific Interest: My research focuses on investigation of advanced functional materials for energy catalytic applications. I am particularly interested in 2D materials such as COFs, MOFs, TMDCs, chalcogenides, and high entropy alloys (HEAs). Using DFT and MD simulations, my work explores catalytic processes, thermoelectric materials, and surface reactions at the atomic scale. The goal is to develop efficient materials for sustainable energy conversion, environmental remediation, and electrochemical catalysis.

Google Scholar ID: <https://scholar.google.com/citations?user=-YGeReQAAAAJ&hl=en>
ORCID; <https://orcid.org/0000-0003-4824-6432>

Academic Qualification

- 2017 – 2021** [PhD, COMSATS University Islamabad, Abbottabad campus, Pakistan
Specialization (Computational Chemistry)
Grade (GPA): 3.54/4
Thesis: Theoretical Studies on Electrochemical Sensing Applications of Nitrogenated Holey Graphene (C₂N) for Toxic Agents
- 2014 – 2017** [M.Phil., HAZARA University Mansehra, Pakistan
Grade (GPA): 3.89/4
- 2003 – 2005** [M.Sc, Bahauddin Zakariya University Multan, Pakistan
Grade (%age): 62.83

Experience : 19 Years

Work Experience

- ❖ **Assistant Professor (BPS-19) at Cholistan University of Veterinary and Animal Sciences (CUVAS) Bahawalpur, Pakistan since 26 March, 2024.**
- ❖ **17 Years as Lecturer in Chemistry**
 - **10 years (3 Nov, 2013 to 25th March, 2024) as lecturer in *Abbottabad Public School & College Abbottabad***
 - **07 years (Sep, 2006 to Oct, 2013) as lecturer in *WAPDA Cadet College, Tarbela.***

Professional Experience:

- ***Officer Incharge Department of Physiology and Biochemistry from Nov, 2024 to June 2026.***
- ***Hostel Warden Cholistan University of Veterinary and Animal Sciences, Bahawalpur, from April 2026 to to-date***

- *Manager Research and Innovation Cholistan University of Veterinary and Animal Sciences, Bahawalpur, from 2024 to to-date*
- *Hostel Warden Abbottabad Public School and College 2023 to 2024*
- *Assistant controller of examination Abbottabad Public school and College Abbottabad from 2017 to 2024*
- *Incharge Admission Branch WAPDA Cadet College Tarbela, Pakistan*

Projects:

1. Transition metal doped on C₂N surface for hydrogen dissociation reaction

[Co-PI, King Faisal University, Grant No. 2125, 2021, SAR 30,000]

2. Role of C₆₀ fullerene towards hydrogen dissociation reaction

[Co-PI, King Faisal University, Grant No. 3861, 2023, SAR 10,000]

3. Hydrogen dissociation reaction via single atom catalysis using transition metals doped on C₂₄ surface

[Co-PI, King Faisal University, Grant No. 2180, 2023, SAR 20,000]

4. Application of graphitic carbon nitride towards development of electrochemical sensor

[Co-PI, King Faisal University, Grant No. 2262, 2023, SAR 20,000]

Communication skills

- Excellent communication and teaching skills.
- Good command of MS office, Linux/Ubuntu

Expertise

- **Density Functional Theory (DFT):**
Gaussian, VASP, Quantum ESPRESSO, ORCA, Psi4
- **Molecular Dynamics (MD):**
GROMACS
- **Semi-Empirical Methods:**
CREST, GFN-xTB, xTB
- **Docking & Modeling:**
AutoDock Vina, Chimera, PyMOL
- **Visualization:**
VMD, ASE
- **Materials Science:**
Pymatgen, Materials Studio
- **Other Tools:**
Multiwfn, ChemCraft, GaussView

Methodologies

- **Conformer Search and Ensemble Generation:** Expertise in identifying stable conformers and exploring potential energy surfaces using tools like CREST and GFN-xTB.
- **Transition State (TS) Location:** Proficient in locating transition states for reaction mechanisms using DFT-based tools (Gaussian, ORCA, and VASP).
- **Band Structure, DOS, and Optical Properties Analysis:** Skilled in calculating and analyzing electronic properties of materials, including band gaps, density of states (DOS), and optical conductivity.
- **Thermochemical and Kinetic Modeling:** Experienced in predicting reaction energies, rates, and mechanisms for various chemical processes.
- **Reaction Mechanism Elucidation:** Deep understanding of reaction pathways and catalytic processes using computational chemistry.
- **Sensors and NLO Materials Design:** Research experience in designing sensors and materials with nonlinear optical properties.
- **Drug Design:** Computational studies for drug binding, docking, and delivery systems.

- **Other Areas of Expertise:** Mechanistic studies of organic reactions, single-atom catalysis, band gap engineering, thermoelectric materials, and surface chemistry using DFT simulations.

Certificate of Excellence: Certificate of Excellence, by Zakariyan Chemist Organization Multan Pakistan, for excellent research in M.Sc. Chemistry.

Professional Trainings / Certificate

International workshop on Computational Biology (August 2-5, 2022)

References

Prof. Dr. Khurshid Ayub (PhD Supervisor)

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Dr Nadeem S. Sheikh (Associate Professor of Organic Chemistry)

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Ph.D (Topic): Theoretical Studies on Electrochemical Sensing Applications of Nitrogenated Holey Graphene (C₂N) for Toxic Agents

Scientific Publications

1. Muhammad Yar, Muhammad Ali Hashmi and Khurshid Ayub*, Nitrogenated holey graphene (C₂N) surface as highly selective electrochemical sensor for ammonia, *Journal of Molecular Liquids*, 2019, 296, 111929 **(IF =5.200)**

(DOI: 10.1016/j.molliq.2019.111929)

2. Muhammad Yar, Muhammad Ali Hashmi, Ayesha Khan and Khurshid Ayub*, “Carbon nitride 2-D surface as a highly selective electrochemical sensor for V-series nerve agents”. *Journal of Molecular Liquids*, 2020, 311, 113357. **(IF =5.200)**

(DOI: 10.1016/j.molliq.2020.113357)

3. Muhammad Yar and Khurshid Ayub*, Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM, *Microporous and Mesoporous Materials*, 2020, 300, 110146. **(IF =4.500)**

(DOI: 10.1016/j.micromeso.2020.110146)

4. Muhammad Yar, Muhammad Ali Hashmi and Khurshid Ayub*, The C₂N surface as high selective sensor for the detection of nitrogen iodide from a mixture of NX₃ (X= Cl, Br, I) explosives, *RSC Advances*, 2020, 10 (53), 31997-32010 **(IF =6.100)**

(DOI: 10.1039/d0ra04930a)

5. Yasir Altaf^a Muhammad Yar^b and Muhammad Ali Hashmi^{*c}, Main-group metal cyclophane complexes with high coordination numbers, *RSC Advances*, 2020, 10, 30796 **(IF =6.100)**

(DOI: 10.1039/d0ra05303a)

6. Bilal Ahmad Farooqi,^a **Muhammad Yar**^b, Ayesha Ashraf,^a Umar Farooq,^a Khurshid Ayub^{b*}, Graphene-polyaniline composite as superior electrochemical sensor for detection of cyano explosives, *European Polymer Journal*, **2020**,138, 109981. (IF = 6.800)

(DOI: 10.1016/j.eurpolymj.2020.109981)

7. Bilal Ahmad Farooqi,^a **Muhammad Yar**,^b Ayesha Ashraf,^a Umar Farooq,^a Khurshid Ayub^{b*}, Remarkable enhancement in sensor ability of polyaniline upon composite formation with ZnO for industrial effluents, *Journal of Molecular Graphics and Modelling*, **2020**,101, 107724. (IF = 3.100)

(DOI: 10.1016/j.jmglm.2020.107724)

8. Hasnain Sajid, Faizan Ullah, **Muhammad Yar**, Khurshid Ayub, Tariq Mahmood, “Superhalogen doping: A new and effective approach to design materials with excellent static and dynamic NLO response”, *New Journal of Chemistry*, **2020**, 44, 16358. (IF = 2.600)

(DOI: 10.1039/d0nj02291h)

9. Sidra Khan, **Muhammad Yar**, Naveen Kosar, Khurshid Ayub, Muhammad Arshad, Nauman Zahid, Tariq Mahmood* “First-principles study for exploring the adsorption behavior of G-series nerve agents on graphyidine surface”, *Computational and Theoretical Chemistry*, **2020**, 11991,113043. (IF = 2.900)

(DOI: 10.1039/d0nj03752d)

10. **Muhammad Yar**, Ahmed Bilal, Muhammad Ali Hashmi and Khurshid Ayub* “Selective detection and removal of picric acid by C₂N surface from a mixture of nitro-explosives” *New Journal of Chemistry*, **44**, 18646-18655, 2020. (IF = 2.600)

(DOI: 10.1039/d0nj03752d)

11. Bilal Ahmad Farooqi, **Muhammad Yar**, Ayesha Ashraf, Umar Farooq, Khurshid Ayub*, “Polyaniline Emeraldine Salt as Selective Electrochemical Sensor for HBr over HCl: A Systematic Density Functional Theory Study through Oligomer Approach. *Journal of Molecular Modeling*, 2020, 26(11):332. (IF = 2.900)

(DOI: 10.1007/s00894-020-04590-3)

12. **Muhammad Yar**, Faiza Ahsan, Adnan Gulzar, Khurshid Ayub*. Adsorption and sensor applications of C₂N surface for G-series and mustard series chemical warfare agents. *Microporous and Mesoporous Materials*, 2021, 317, 110984. (IF = 4.500)

(DOI: 10.1016/j.micromeso.2021.110984)

13. Zulqurnain Chaughtai, M. Ali Hashmi, **Muhammad Yar**, Khurshid Ayub* Electronic structure of polypyrrole composited with low percent of graphene nanofiller. *Phys. Chem. Chem. Phys.*, **2021**,23, 8557-8570. (IF = 3.000)

(DOI: 10.1039/D0CP03258A)

14. Maryum Munir#, **Muhammad Yar**#, Faiza Ahsan and Khurshid Ayub* Unprecedented saturation limit achieved by inorganic polycationic cluster (Sb₇Te₈)⁵⁺ for light noble gases (He & Ne). *Journal of Molecular Graphics and Modelling*, **2021**, **106**, 107910. (IF = 3.100)

(DOI: 10.1016/j.jmglm.2021.107910)

15. Faiz Rasool, Muhammad Khalid, **Muhammad Yar**, Khurshid Ayub, Muhammad Tariq, Ajaz Hussain, Mehreen Lateef, Muhammad Kashif, Sana Iqbal. “Facile synthesis, DNA binding, Urease inhibition, anti-oxidant, molecular docking and DFT studies of 3-(3-Bromo-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone and 3-(3-Bromo-5-chloro-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone”. *Journal of Molecular Liquids*, **2021**,336, 116302. (IF = 5.200)

(DOI: 10.1016/j.molliq.2021.116302)

16. Muhammad Hamid Butt, Syeda Huda Mehdi Zaidi, Ayesha Khan, Khurshid Ayub, **Muhammad Yar**, Muhammad Ali Hashmi, Mirza Arfan Yawer, Muhammad Abid Zia. "Cu-doped phosphorene as highly efficient single atom catalyst for CO oxidation: A DFT study. *Molecular Catalysis*, **2021**, 509, 111630. (IF= 4.300)

(DOI: 10.1016/j.mcat.2021.111630)

17. Muhammad Tariq, Rabbia Khan, Ajaz Hussain, Atia Batool, Faiz Rasool, **Muhammad Yar**, Khurshid Ayub, Muhammad Sirajuddin, Faizan Ullah, Saqib Ali, Arusa Akhtar, Samia Kausar Ataf Ali Altaf. Synthesis, characterization, antimicrobial, cytotoxic, DNA-interaction, molecular docking and DFT studies of novel di- and tri-organotin (IV) carboxylates using 3-(3-nitrophenyl)2-methylpropenoic acid. *Journal of Coordination Chemistry*, **2021**, 317, 110984. (IF= 1.600)

(DOI: 10.1080/00958972.2021.1964019)

18. Satenik Mkrtchyan, Michał Jakubczyk, Suneel Lanka, **Muhammad Yar**, Khurshid Ayub, Mohanad Shkoor, Michael Pittelkow, Viktor Iaroshenko. "Mechanochemical transformation of CF₃ group: Synthesis of amides and Schiff bases". *Advanced Synthesis & Catalysis*, **2021**, 363, 1-14 (IF= 3.700)

(DOI: 10.1002/adsc.202100538)

19. Sehrish Sarfaraz#, **Muhammad Yar**#, & Khurshid Ayub*, "Covalent triazine framework (CTF-0) surface as a smart sensing material for the detection of CWAs and industrial pollutants". *Materials Science in Semiconductor Processing*, **2022**, 139, 106334. (IF = 5.200)

(DOI: 10.1016/j.mssp.2021.106334)

20. Faiz Rasool, Ajaz Hussain, Khurshid Ayub, Muhammad Tariq, Khalid Mahmood, Sammer Yousuf, **Muhammad Yar**, Muhammad Khalid, Hafiza Saba Samreen, Mehreen Lateef, Abdul Malik, "Experimental and Theoretical investigations on (E)-3-(4-ethoxyphenyl)-1-(2-(trifluoromethyl)phenyl)prop-2-en-1- (E)-3-(naphthalen-2-yl)-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-one: DNA binding, Urease inhibition and Promising NLO response" *Journal of Molecular Structure*, 2022,1253, 132194. (IF = 4.900)

(DOI: 10.1016/j.molstruc.2021.132194 0022-2860)

21. Iram Gul, **Muhammad Yar**, Arsalan Ahmed, Muhammad Ali Hashmi, Khurshid Ayub. Permeability of Boron and Nitrogen Doped Graphene Nanoflakes for Protium/Deuterium Ions *RSC Adv.*, 2022,12, 3883-3891. (IF =6.100)

(DOI: 10.1039/D1RA09398C)

22. Sehrish Sarfaraz#, **Muhammad Yar**#, Muhammad Ans, Mazhar Amjad Gilani, Ralf Ludwig, Muhammad Ali Hashmi, Masroor Hussain, Shabbir Muhammad, & Khurshid Ayub*. Computational investigation of covalent triazine framework (CTF-0) as an efficient electrochemical sensor. *RSC Adv.*, 2022, 12, 3909 (IF =6.100)

(DOI: 10.1039/D1RA08738J)

23. Sehrish Sarfaraz, **Muhammad Yar**, Adnan Ali Khan, Rashid Ahmad, & Khurshid Ayub*. DFT investigation of adsorption of nitro-explosives over C₂N surface: highly selective towards trinitro benzene. *Journal of Molecular Liquids*.352, 15 April **2022**, 118652. (IF =5.200)

(DOI: 10.1016/j.molliq.2022.118652)

24. Faiza Ahsan, **Muhammad Yar**, Adnan Gulzar, and Khurshid Ayub*. Therapeutic potential of C₂N as targeted drug delivery system for fluorouracil and nitrosourea to treat cancer: A theoretical study. *J Nanostruct Chem* (2022). 022-00474-5. (IF = 7.300)

(DOI: 10.1007/s40097-022-00474-5)

25. Faiza Fayyaz, **Muhammad Yar**, Adnan Gulzar, Khurshid Ayub, First principles calculations of the adsorption of fluorouracil and nitrosourea on CTF-0; organic frameworks as drug delivery systems for cancer treatment. *Journal of Molecular Liquids*. 356, (2022) 118941. (IF =5.200)

(DOI: 10.1016/j.molliq.2022.118941)

26. Qaisar Ali, Adnan Ali Khan, **Muhammad Yar**, Momin Khan, Rashid Ahmad, Iftikhar Ahmad. Theoretical insight of ciprofloxacin removal from water using boron nitride (B₁₂N₁₂) nanocage, *Surfaces and Interfaces*. 31, 101982, 2022. (IF = 6.000)

(DOI: 10.1016/j.surfin.2022.101982)

27. Faiz Rasool, Ajaz Hussain*, **Muhammad Yar**, Khurshid Ayub, Muhammad Sajid, Muhammad Ali Khan, Hafiz Muhammad Asif, Muhammad Imran. Nonlinear Optical Response of 9,10-bis(phenylethynyl)anthracene mediated by electron donating and electron withdrawing substituents: A Density Functional Theory approach. *Materials Science in Semiconductor Processing*. 148, 106751, 2022 (IF = 5.200)

(DOI: 10.1016/j.mssp.2022.106751)

28. Maryam Munir#, Faiza Ahsan#, **Muhammad Yar**, and Khurshid Ayub*. Theoretical investigation of double-cubed polycationic cluster (Sb₇Se₈Cl₂)³⁺ for the storage of helium and neon. *Materials Science in Semiconductor Processing*. 148, 106756, 2022 (IF = 5.200)

(DOI: 10.1016/j.mssp.2022.106756)

29. Satenik Mkrtchyan, Michał Jakubczyk, Suneel Lanka, **Muhammad Yar**, Tariq Mahmood, Khurshid Ayub, Mika Sillanpää, Christine Thomas., Viktor Iaroshenko. Mechanochemical Ni-catalysed arylation of ortho-hydroxyarylenaminones: Synthesis of isoflavones. *Adv. Synth. Catal.* 2022, 364, 1 –11. (IF = 3.700)

(DOI: 10.1002/adsc.202200645)

30. Sania bibi, Sehrish Sarfaraz, **Muhammad Yar**, Muhammad Iqbal Zaman, Abdul Niaz, Muhammad Ali Hashmi, Ayesha Khan. Structure and electronic characterization of pristine and functionalized single wall carbon nanotube interacting with sulfide ion: A density functional theory approach. *Journal of Molecular Liquids*. 366, 2022, 120144 (IF =5.200)

(DOI: 10.1016/j.molliq.2022.120144)

31. Mohammed A. Alkhalifah ^{1,*}, **Muhammad Yar** ², Imene Bayach ¹, Nadeem S. Sheikh ³ and Khurshid Ayub ^{2,*}. Covalent organic framework (C₆N₆) as a drug delivery platform for fluorouracil to treat cancerous cells. *Materials*, 15, 7425, 2022. (IF=3.700)

(DOI: 10.3390/ma15217425)

32. Ahmed Bilal Shah¹, Sehrish Sarfaraz¹, **Muhammad Yar**¹, Nadeem S. Sheikh², Hassan H. Hammud^{3,*} Khurshid Ayub ^{1,*}. Remarkable Single Atom Catalyst of Transition Metal (Fe, Co & Ni) Doped on C₂N Surface for Hydrogen Dissociation Reaction. *Nanomaterials* 2022, 12. (IF=4.800)

(DOI: 10.3390/nano13010029)

33. Yasair S. S. Al-Faiyz* Sehrish Sarfaraz, **Muhammad Yar**, Sajida Munsif, Adnan Ali Khan, Bin Amin, Nadeem S. Sheikh, and Khurshid Ayub*. Efficient Detection of Nerve Agents through Carbon Nitride Quantum Dots: A DFT Approach. *Nanomaterials*. 2023, 13, 251. (IF=4.800)

(DOI: 10.3390/nano13020251)

34. Muniba Iqbal Ajaz Hussain Asma Aziz Riaz Hussain **Muhammad Yar*** Khurshid Ayub M. Rehan H. Shah Gilani Muhammad Imran Mohammed A. Assiri. Tailoring the solar cell efficiency of Y-series based non-fullerene acceptors through end cap modification. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. 2023, 291, 122322. (IF=4.800)

(DOI: 10.1016/j.saa.2023.122322)

35. Rasool, Faiz and Hussain, Ajaz and Rizvi, Tania Shamim and **Yar, Muhammad** and Ayub, Khurshid and Khalid, Muhammad and Al-Harrasi, Ahmad and Lateef, Mehreen and Iqbal, Sana. Combined experimental and computational approach toward biological, physicochemical and quantum chemical aspects of substituted 1-[5-Phenyl-3-(2-trifluoromethyl-phenyl)-4,5-dihydro-pyrazol-1-yl]-ethanone. *Results in Chemistry*. 5 (2023) 100772. (IF=5.800)

(DOI: 10.1016/j.rechem.2023.100772)

36. Yasir Arshad, Maria Asghar, **Muhammad Yar**, Tamseela Bibi, and Khurshid Ayub*. Transition Metal Doped Boron Nitride Nanocages as High Performance Nonlinear Optical Materials. A DFT Studies. *Journal of Inorganic and Organometallic Polymers and Materials*. 2023, 7, 02546 (IF=6.000)

(DOI: 10.1007/s10904-023-02546-7)

37. Sehrish Sarfaraz, **Muhammad Yar**, Riaz Hussain, Khurshid Ayub* Adsorption and dissociation of H₂ molecule over first-row transition metal doped C₂₄ nanocage as remarkable SACs: A comparative study. *International Journal of Hydrogen Energy*, Volume 48, Issue 54, 29 June 2023, Pages 20633-20645 (IF=9.200)

(DOI: 10.1016/j.ijhydene.2023.03.018)

38. Hassan H. Hammud^{1,*},[†], **Muhammad Yar** ^{2,†}, Imene Bayach¹ and Khurshid Ayub ^{2,*}. Covalent Triazine Framework C₆N₆ as an Electrochemical Sensor for Hydrogen-Containing Industrial Pollutants. A DFT Study. *Nanomaterials*, 2023, 13, 1121. (IF=4.800)

(DOI: 10.3390/nano13061121)

39. Sarfaraz, Sehrish; **Yar, Muhammad**; Sheikh, Nadeem; Bayach, Imene; Ayub, Khurshid. Transition metal doped C₂₀ fullerene-based SACs with high catalytic activity for hydrogen dissociation reaction. *ACS Omega*. 2023, 8, 15, 14077–14088 (IF=5.200)

(DOI: 10.1021/acsomega.3c00721)

40. Sayed Zahid Nasim, Sehrish Sarfaraz, Faheem Jan*, **Muhammad Yar***, Attiq Ur Rehman. Computational Insights of Excited State Intramolecular Proton Transfer (ESIPT) Based Fluorescent Detection and Imaging of γ -Glutamyltranspeptidase Activity. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. 299 (2023) 122814 (IF=4.800)

(DOI: 10.1016/j.saa.2023.122814)

41. Muniba Iqbal¹, Ajaz Hussain*, Riaz Hussain, Khurshid Ayub, **Muhammad Yar**, Faiz Rasool, Muhammad Imran, Mohammed A. Assiri, Abdul Sattar. Computational perspective of Benzo-thiadiazole based molecules as an alternate promising non-fullerene acceptor for organic solar cells. *Solar energy*. 2023, 260, 34-48 (IF=7.900)

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42. Satenik Mkrtchyan*, Vishal B. Purohit, Spartak Khutsishvili, Jela Nociarova, **Muhammad Yar**, Tariq Mahmood, Khurshid Ayub, Simon Budzak, Marek Skoršepa, Viktor O. Iaroshenko.*. Mechanochemical defluorinative acylation of ortho-hydroxyarylenaminones by CF₃–compounds: Synthesis of 3-acylchromones. *Adv. Synth. Catal.*2023, 365, 1–1 (IF= 3.700)

(DOI: 10.1002/adsc.202300260)

43. Satenik Mkrtchyan, Vishal B. Purohit, Sehrish Sarfaraz, **Muhammad Yar**, Khurshid Ayub and Viktor O. Iaroshenko*. Metal-Free Supramolecular Reduction of Nitro Compounds into the Cucurbit[7]uril Cavity: Testing the Enabling Technique in Aqueous Media. *ACS Sustainable Chem. Eng.* 2023, 11, 8406–8412 (IF= 7.600)

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44. Hafiza Saba Samreen, Ajaz Hussain, **Muhammad Yar**, Mohammed Battah Alshammari, Khurshid Ayub, Muhammad Adeel, Muhammad Tariq, Mehreen Lateef, Mohammed Afroz Bakht, Faiz Rasool. Photophysical and Biological aspects of α , β -unsaturated Ketones: Experimental and in silico approach". *Journal of Biochemical and Molecular Toxicology*. Volume 37, Issue 10. October 2023. e23433. (IF= 3.600)

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45. Maria Younas, **Muhammad Yar**, Hamad AlMohamadi, Tariq Mahmood, Khurshid Ayub, Asim Laeeq Khan*, Muhammad Yasin, Mazhar Amjad Gilani*. A Rational Design of Covalent Organic Framework Supported Single Atom Catalysts for Hydrogen Evolution Reaction: A DFT Study. *International Journal of Hydrogen Energy*. Volume 51, Part A, 2 January 2024, Pages 758-773. (IF=9.200)

(DOI: 10.1016/j.ijhydene.2023.07.062)

46. Sehrish Sarfaraz, **Muhammad Yar**, Ahmed Lakhani*, Nadeem S. Sheikh, Imene Bayach* & Khurshid Ayub* Probing the catalytic activity of first-row transition metal doped C20 fullerene as remarkable HER electrocatalysts: A DFT study. *Materials Science in Semiconductor Processing* (2023). 167, 2023, 107785. (IF = 5.200)

(DOI: 10.1016/j.mssp.2023.107785)

47. Sehrish Sarfaraz, **Muhammad Yar**, Khurshid Ayub*. The electronic properties, stability and catalytic activity of metallofullerene (M@C60) for robust hydrogen evolution reaction: DFT insights. *International Journal of Hydrogen Energy*. Volume 51, Part B, 2 January 2024, Pages 206-221. (IF=9.200)

(DOI: 10.1016/j.ijhydene.2023.08.123)

48. Sehrish Sarfaraz, **Muhammad Yar**, Ajaz Hussain, Ahmed Lakhani, Adnan Gulzar, Muhammad Ans, Umer Rashid, Masroor Hussain, Shabbir Muhammad, Imene Bayach, Nadeem Sheikh, Khurshid Ayub, "Metallofullerenes as robust single atom catalysts for adsorption and dissociation of hydrogen molecule: A density functional study". *ACS Omega*. 2023, 8, 39, 36493–36505. (IF=5.200)

(DOI: 10.1021/acsomega.3c05477)

49. Sehrish Sarfaraz, **Muhammad Yar**, Muhammad Umair Ashraf & Khurshid Ayub* "Highly efficient transition metal doped C24 electrocatalysts for hydrogen evolution reaction: Kinetic and thermodynamic aspects". *Materials Science in Semiconductor Processing*. Volume 168, December 2023, 107840. (IF = 5.200)

(DOI: 10.1016/j.mssp.2023.107840)

50. Sabra Yousaf a, Talal Akhtar a, Najla AlMasoud b, Khurshid Ayub c, Sana Rauf d, Muhammad Tariq a, **Muhammad Yar** c, Taghrid S. Alomar b, Hafiz Muhammad Asif a, Zeinhom M. El-Bahy. Porphyrin-Anhydride Co-Sensitization Strategy for Enhanced Photovoltaic Performance in DSSC: A Combined Experimental and Theoretical Approach. *Polyhedron*. Volume 246, 1 December 2023, 116675. (IF =2.800)

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51. Aleena Mustafai", "**Muhammad Yar***", "Riaz Hussain", "Khurshid Ayub", "Muhammad Imran", "Mohammed A. Assiri" Triquinoxalinylene and Benzoquinone based Covalent Organic Framework as robust material for mitigation of environmental pollutants-A theoretical approach. *Journal of Molecular Liquids*. Volume 391, Part B, 1 December 2023, 123304 (IF =5.200)

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52. "Sadia Farooq "**Muhammad Yar**", "Muhammad Tariq", "Khalid Mahmood", "Khurshid Ayub", "Riaz Hussain", "Faiz Rasool", "Muhammad Imran", "A.Assiri Mohammed" Nonlinear optical response of facially polarized all cis-1,3,5-trifluorocyclohexane doped with transition metals and calcium. *Journal of Molecular Liquids*. Volume 391, 2023, 123331 (IF =5.200)

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