Dr Muhammad Ali Hashmi

Assistant Professor Department of Chemistry University of Education Lahore, Attock Campus, Attock, Pakistan +923455341331, <u>i4hashmi@hotmail.com</u>, <u>muhammad.hashmi@ue.edu.pk</u>

RESEARCH INTERESTS

Drug Delivery through Ionic Liquids and other Nano-Careers, Hydrogen Evolution Reaction through Single-Atom Catalysis, Oxidation of CO and CO₂, Electrochemical Sensors, conformational analysis of flexible systems and their physical properties, prediction of accurate NMR spectra using computational chemistry tools, mechanistic investigation of organic synthetic pathways.

TEACHING and RESEARCH EXPERIENCE

(March 2019 – present)	Assistant Professor, University of Education Lahore, Attock Campus
	Campus Coordinator (HoD) for Chemistry Department
	 Teaching chemistry courses to BS and MS Chemistry Students
	Supervising BS Chemistry Labs
	 Supervising BS and MS students' theses
	Incharge Student Affairs (2019-21)
(Oct 2018 – March 2019)	Assistant Professor, University of Management & Technology, Lahore
	• Teaching Principles of Chemistry I (CH-101) to BS students.
	Teaching "Theoretical & Computational Chemistry" to BS Students
	Supervising Principles of Chemistry I (CH-101) labs.
	Supervising Organic Chemistry (CH-206) labs.
	Supervised 3 MS students' theses
(Nov 2017 – Aug 2018)	Research Assistant, Victoria University of Wellington, New Zealand
	 Big data analysis on Wikipedia edits using Python programming language and high-performance computing.
(2015 – 2017)	Lab Demonstrator, Victoria University of Wellington, New Zealand
	• Demonstrating and supervising laboratory experiments to university students (CHEM113 and CHEM114) and marking their assignments
	 Demonstrating and supervising the computational chemistry lab to 3rd year university students (CHEM306)
(2015 – 2017)	Doctoral research, Victoria University of Wellington, New Zealand
	• Computational studies for the structure revision and absolute configuration of echivulgarine, a pyrrolizidine alkaloid.

	• Development of a tool for accurately mapping of the potential energy surface of a flexible molecule, called <i>MICE-PES</i> .
	• Structural validation of 3-epi-xestoaminol C and meroterphenol C.
	• Studies of structure and electronic properties of carbon nano-onions.
	• Tracking the source of enantioselectivity in the reaction between the enantiomers of 2-formyl-3-hydroxyl[2.2]paracyclophane (FHPC) with (S)-valyl-(S)-valine using density functional theory (DFT).
	Mechanistic studies of some organic reactions.
(2012 – 2015)	Doctoral research, COMSATS IIT, Abbottabad, Pakistan
	• Isolation of chemical constituents of the indigenous medicinal plant, <i>Olea ferruginea</i> using silica gel column chromatography and thin layer chromatography.
	Purification of the isolated compounds using semi-preparative HPLC
	 Characterization of pure compounds using various spectroscopic techniques including ESI-MS, EI-MS, IR, UV-Vis, ¹H-NMR, ¹³C-NMR, and 2D-NMR techniques.
	• Quantum chemical studies of properties of some small sized natural products.
(March-Aug – 2010)	Vice Principal – Base School System, Gujar Khan, Pakistan
	Delivering lectures to secondary school chemistry students.
	• Teaching and demonstrating the laboratory experiments to the students.
	• Setting up and marking assignments and examination papers.
	Looking into disciplinary matters
	• Holding meetings with teachers and students' parents, and resolving the conflicts, if any.
(2009 – 2010)	Chemistry Lecturer – Indus Group of Colleges, Gujar Khan, Pakistan
	• Delivering lectures to higher secondary school chemistry students.
	• Teaching and demonstrating the laboratory experiments to the students.
	• Setting up and marking assignments and examination papers.
Editorial and Reviewer Ex	perience
(Dec 2020 – present)	Academic Editor, Evidence-Based Complementary and Alternative
	Medicine
	Handling of the manuscripts assigned to me for their initial assessment
	Sending out the manuscripts for peer-review
	 Making decisions about the publication of manuscripts after the peer- review process

(Dec 2018 – present)	Reviewer of the following Scientific Journals
	 Molecular Catalysis RSC Advances Computational and Theoretical Chemistry International Journal of Quantum Chemistry Crystals (MDPI) Energy (MDPI) Frontiers in Nutrition Journal of Taibah University for Science Evidence-Based Complementary and Alternative Medicine Journal of Traditional and Complementary Medicine Biomedicine & Pharmacotherapy
EDUCATION	
(2018)	PhD in Chemistry, Victoria University of Wellington, New Zealand
	<u>Area of Research</u> : Theoretical and Computational Chemistry <u>Dissertation</u> : MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products.
(2016)	PhD in Chemistry, COMSATS IIT, Abbottabad, Pakistan
	<u>Area of Research</u> : Natural Product Chemistry <u>Dissertation</u> : Phytochemical Investigation of Bioactive Compounds from Olea ferruginea and Quantum Chemical Studies of Important Natural Products.
(2012)	MS in Chemistry, COMSATS IIT, Abbottabad, Pakistan
	<u>Dissertation</u> : Isolation and Characterization of Chemical Constituents of Olea ferruginea.
(2009)	MSc in Chemistry, The University of Azad Jammu & Kashmir, Muzaffarabad, Pakistan
	Dissertation: NMR Studies of Isoquinoline Alkaloids.
(2006)	B.Sc. in Chemistry, University of the Punjab, Lahore, Pakistan

HONOURS AND AWARDS

(2014)	Victoria Doctoral Scholarship
(2014)	CAS/TWAS President's PhD Scholarship (Not Availed)
(2014)	COMSATS IIT Research Productivity Award (2013 and 2014)
(2012)	3 rd Prize for Poster Presentation at 3rd International Symposium on
	Biomedical Materials: Advances and Challenges (December 18-19)
(2011)	Higher Education Commission of Pakistan's Indigenous PhD Fellowship
(2010)	COMSATS IIT Merit Scholarship for MS Studies

TECHNICAL SKILLS

- Experienced in high performance computing, use of computational chemistry software including Gaussian, ORCA, GaussView, ChemCraft etc.
- Advanced user of Python programming language.
- Highly experienced in the isolation and characterization of chemical compounds from natural products using different chromatographic techniques (column, size exclusion, thin layer, and high-pressure liquid chromatography (HPLC)) and spectroscopic techniques including mass spectrometry, NMR spectroscopy, UV-Vis, and IR spectroscopy.
- Experience of working with recycling preparative grade HPLC.
- Excellent written and communication skills in English (IELTS band score of 7.5).
- Excellent scientific writing skills (authored >60 research articles in peer-reviewed international journals).
- Experienced in research grants proposal writing.
- Proficient with Windows, MAC, and Linux operating systems. Advanced user of computer applications including Microsoft office suite, ChemBio Office, LaTeX, GNU-Plot, Endnote, and Adobe Photoshop.

CONFERENCES

 for CO Oxidation", 2nd International Conference of Sciences "Revamped Scientific Outlook of 21st Century, 2023", Rawalpindi Women University, (November 15–16 2023). (2020) <u>Muhammad Ali Hashmi</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Reaction Using Transition Metals on Phosphorene Support", 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry-CCUMT-2019 Lahore, Pakistan, (November 27–29) 	C
 (2020) Outlook of 21st Century, 2023", Rawalpindi Women University, (November 15–16 2023). (2020) <u>Muhammad Ali Hashmi</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Reaction Using Transition Metals on Phosphorene Support", 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry-CCUMT-2019 Lahore, Pakistan, (November 27–29) 	,
 (2020) <u>Muhammad Ali Hashmi</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Reaction Using Transition Metals on Phosphorene Support", 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry-CCUMT-2019 Lahore, Pakistan, (November 27–29) 	
 (2020) <u>Muhammad Ali Hashmi</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Reaction Using Transition Metals on Phosphorene Support", 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Lahore Pakistan (November 27–29) 	
 Hydrogen Evolution Reaction Using Transition Metals on Phosphorene Support", 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Lahore, Pakistan, (November 27–29) 	
 1st International Conference on Advances in Materials Science - AIMS-2020, University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Lahore, Pakistan, (November 27–29) 	
 University of Education Lahore, Pakistan, (July 23–24). (2019) <u>Muhammad Ali Hashmi</u>, Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30th Nation & 18th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Lahore, Pakistan, (November 27–29) 	
(2019) <u>Muhammad Ali Hashmi</u> , Matthias Lein, "MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products", 30 th Nation & 18 th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Labore Pakistan (November 27–29)	
Conformational Analysis and its Implementation to Natural Products", 30 th Nation & 18 th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Labore Pakistan (November 27–29)	
& 18 th International Chemistry Conference on Recent Trends in Chemistry- CCUMT-2019 Labore Pakistan (November 27–29)	al
CCUMT-2019 Labore Pakistan (November 27–29)	
(2017) <u>Muhammad Ali Hashmi</u> , Matthias Lein, "Conformational Analysis and Accurate	
Prediction of Molecular Properties for Highly Flexible Chiral Natural Products",	
World Association of Theoretical and Computational Chemists (WATOC)	
Chemistry Congress, Munich, Germany, (August 26 – September 01, 2017).	
(2016) <u>Muhammad Ali Hashmi</u> , Robert A. Keyzers, Matthias Lein, "Accurate prediction	of
the optical rotation and NMR properties for highly flexible chiral natural products"	,
NZIC International Chemistry Conference, Queenstown, New Zealand, (August	
21–24, 2016).	
(2014) <u>Muhammad Ali Hashmi</u> , "A New Secoirridoid Glycosidic Lignan Ester from the	
Leaves of Olea ferruginea", 13th International and 25th National Chemistry	
Conference of the Chemical Society of Pakistan, University of the Punjab, Lahore	Э,
Pakistan (October 20–22, 2014).	

(2013)	Muhammad Ali Hashmi, "Spectroscopic and Density Functional Theory Studies of
	5,7,3',5'-Tetrahydroxyflavanone isolated from the Leaves of Olea ferruginea", 12 th
	International and 24th National Chemistry Conference, Bahauddin Zakariya
	University, Multan, Pakistan (October 28-30, 2013).
(2012)	Muhammad Ali Hashmi, Aisha Hameed, Afsar Khan, "A New Diarylheptanoid from
	the Male Flowers of Alnus nitida", 3rd International Symposium on Biomedical

the Male Flowers of Alnus nitida", 3rd International Symposium on Biomedical Materials: Advances and Challenges, Interdisciplinary Research Center for Biomedical Materials, CIIT Lahore, Pakistan (December 18-19, 2012).

MS STUDENTS' THESIS SUPERVISED (11 Thesis)

(2019) <u>Adeel Mubarik</u>, "Computational studies of selected benzothiazole and thiophene sulfonamide derivatives", November 2019 – GC University Faisalabad, Faisalabad, Pakistan – (Co-Supervisor)

(2020) <u>Muhammad Hamid Butt</u>, "A Computational Study of Single-Atom Catalysis of CO Oxidation Using Transition Metal Embedded Phosphorene Support", August 2020 – University of Management & Technology, Lahore, Pakistan

(2020) <u>Sonia Iqbal</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Using Transition Metal on Phosphorene Support", March 2020 – University of Management & Technology, Lahore, Pakistan

(2020) <u>Kainat Hira</u>, "Computational Study of Single-Atom Catalysis of Hydrogen Evolution Using Transition Metal Embedded Boron Nitride Support", March 2020 – University of Management & Technology, Lahore, Pakistan

(2021) <u>Sahar Ishaq</u>, "Density Functional Theoretical Study of Octacyclic Naphto [1, 2-b: 5, 6-b] Dithiophene Based Electron Acceptors for Organic Solar Cells", February 2021 – University of Education Lahore, DG Khan Campus, DG Khan, Pakistan – (Co-Supervisor)

(2023) <u>Syeda Huda Mehdi Zaidi</u>, "A C₅N₂ Nanoparticles Based Drug Delivery System for Anticancer Drugs: A DFT Study", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2023) <u>Nisha Asghar</u>, "Computational Investigation of Carbon Nitride as an Electrochemical Sensor for Toxic Chemicals", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2023) <u>Adeela Naz</u>, "A DFT Study of Electrocatalytic Properties of Heteroatom Doped Phosphorene for Hydrogen Evolution Reaction", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2023) <u>Rimsha Niaz</u>, "A DFT Study of Electrocatalytic Properties of Heteroatom Doped Germanene for Hydrogen Evolution Reaction", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2023) <u>Nabeela</u>, "Computational Investigation of Carbon Nitride as an Electrochemical Sensor for Nitro-Aromatics", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2023) <u>Saleha Asghar</u>, "Utilization of Different Low-Cost Biosorbents for the Removal of Congo Red Dye from Aqueous Solutions", July 2023 – University of Education Lahore, Attock Campus, Attock, Pakistan

BS STUDENTS' THESIS SUPERVISED (11 Thesis)

(2022) <u>Alisha Sultan</u>, "Investigation of the Binding Affinity of Metal Pollutants Towards Bacillibactin: A DFT Study", July 2022 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2022) <u>Fatima Yaseen</u>, "A Computational Study of Hydrogen Evolution Reaction Using Electrocatalysis on Transition Metal-Corrole Complexes", July 2022 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2022) <u>Qurat UI Ain</u>, "A Computational Study on Single-Atom Catalysis of CO Oxidation via Eley Rideal Mechanism Using Mn-Corrole Catalyst", July 2022 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2022) <u>Muhammad Shaheer Kiani</u>, "Investigation of the Binding Affinity of Metal Pollutants Towards Chrysobactin: A DFT Study", July 2022 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2022) <u>Shahab Jilani</u>, "Computational Study on Single-Atom Catalysis of CO2 Reduction via Bi-Molecular Mechanism using Cu-adsorbed Phosphorene", July 2022 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Syeda Huda Mehdi Zaidi</u>, "A Computational Study of Single-Atom Catalysis of CO Oxidation via Langmuir-Hinshelwood Mechanism Using Cu-Doped Phosphorene", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Nabeela</u>, "A Computational Study of Single-Atom Catalysis of CO Oxidation via Eley-Rideal Mechanism Using Cu-Doped Phosphorene", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Zainab Rasheed</u>, "A Computational Investigation of Removal of Toxic Metals (As, Pb, Hg, Cd) from Aqueous Solutions Using Enterobactin", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Tooba Kainat</u>, "A Computational Investigation of Removal of Toxic Metals (Cr, Ni, Cu, Zn) from Aqueous Solutions Using Enterobactin", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Khursheed Ahmed</u>, "A Computational Study of Single-Atom Catalysis of Hydrogen Evolution Reaction Using Ni-Doped Phosphorene", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

(2021) <u>Saleha Asghar</u>, "Determination of Absolute Configuration of Ballonigrin lactone A using DFT Calculations", July 2021 – University of Education Lahore, Attock Campus, Attock, Pakistan

PUBLICATIONS

(Based on JCR 2022, cumulative Impact Factor (I. F.) of 66 published & accepted papers: 224.5)

Year 2024

- Fatima Yaseen, <u>Muhammad Ali Hashmi*</u>, Qurat Ul Ain, Ahmed Lakhani, Khurshid Ayub, "The First Row Transition Metal-Corrole Complexes as a Single Atom Catalyst for Electrochemical Hydrogen Evolution Reaction: A DFT Insight", *International Journal of Hydrogen Energy*, **2024**, 57, 1389-1397 (DOI: <u>10.1016/j.ijhydene.2024.01.135</u>). (I.F. 7.2)
- 2). Zubi Sadiq, Ambreen Ghani, <u>Muhammad A. Hashmi</u>, A. Dahshan, Shahnaz, Samiah H. Al-Mijalli, Munawar Iqbal, Erum Akbar Hussain, "Green synthesis of novel spiropyrazoline-indolinones in neutral deep eutectic solvents and DFT studies", *Heliyon*, 2024, 10, e23814 (DOI: <u>10.1016/j.heliyon.2023.e23814</u>). (I.F. 4.0)

<u>Year 2023</u>

- Amna Ayub, <u>Muhammad Ali Hashmi*</u>, Haq Nawaz Bhatti, Yasir Jamil, Javed Iqbal, "Effect of Binding Pockets on the Kinetics and Thermodynamics of Diels-Alder Reaction in Cucurbit-Uril Family", *Journal* of Molecular Structure, 2023, 1296, 136833 (DOI: <u>10.1016/j.molstruc.2023.136833</u>). (I.F. 3.8)
- Qurat UI Ain, <u>Muhammad Ali Hashmi*</u>, Amna Ayub, Ahmed Lakhani; Khurshid Ayub, "Theoretical Investigation of the CO oxidation mechanism over Mn-Corrole as a Single Atom Catalyst", *Materials Science in Semiconductor Processing*, 2024, 169, 107905 (DOI: <u>10.1016/j.mssp.2023.107905</u>). (I.F. 4.1)
- 5). Saeed Anwar, Wajid Rehman, Rafaqat Hussain, Shoaib Khan, Mohammed M. Alanazi, Nawaf A. Alsaif, Yousaf Khan, Shahid Iqbal, Adeela Naz, <u>Muhammad Ali Hashmi</u>, "Investigation of Novel Benzoxazole-Oxadiazole Derivatives as Effective Anti-Alzheimer's Agents: *In Vitro* and *In Silico* Approaches", *Pharmaceuticals*, 2023, 16(7), 909 (DOI: 10.3390/ph16070909). (I.F. 4.6)
- Maria Asghar, Ahmed Lakhani, Misbah Asif, Nadeem S. Sheikh, <u>Muhammad Ali Hashmi</u>, Ralf Ludwig, Hassan H. Hammud, Khurshid Ayub, "Chiral Recognition of Amino acids using CC₂ Porous Organic Cage", *Journal of Physical Chemistry A*, **2023**, *127*(19), 4245-4258 (DOI: <u>10.1021/acs.jpca.2c08859</u>). (I.F. 2.9)
- 7). Muhammad Hamid Butt, Qurat Ul Ain, Ahmed Lakhani; Mirza Arfan Yawer, <u>Muhammad Ali Hashmi*</u>, "Carboxyl substituted Bambus[6]uril as a Novel Macrocyclic Receptor for Cyanide Anion: A DFT Study", *Computational and Theoretical Chemistry*, **2023**, *1222*, 114081 (DOI: j.comptc.2023.114081). (I.F. 2.8)
- Misbah Naeem, Saleha Asghar, Umar Farooq, Ahmed Lakhani, Yasir Altaf, <u>Muhammad Ali Hashmi*</u>, "Determination of Absolute Configuration of Ballonigrin Lactone A Using Density Functional Theory Calculations", ACS Omega, 2023, 8(2), 1923-1928. (DOI: <u>10.1021/acsomega.2c03858</u>). (I.F. 4.1)
- 9). Sonia Iqbal, Khursheed Ahmed, Khurshid Ayub, Muhammad Hamid Butt, Ahmad Nauman Shah Saqib, Ahmed Lakhani, Ch. Muhammad Fahim Ayaz, <u>Muhammad Ali Hashmi*</u>, "Transition Metals Incorporated on Phosphorene Sheet as Cost-Effective Single Atom Catalysts for Hydrogen Evolution Reaction: A DFT Study", *Computational and Theoretical Chemistry*, 2023, 1220, 113998-114003 (DOI: <u>10.1016/j.comptc.2022.113998</u>). (I.F. 2.8)

<u>Year 2022</u>

10).Amna Ayub, Muhammad Ans, Sehrish Gul, Ahmed M. Shawky, Khurshid Ayub, Javed Iqbal, <u>Muhammad Ali Hashmi</u>, Ahmed Lakhani, "Toward High-Performance Quinoxaline Based Nonfullerene Small Molecule Acceptors for Organic Solar Cells", *Electronic Materials Letters*, 2022, 19, 38-54 (DOI: <u>10.1007/s13391-022-00378-0</u>). (I.F. 2.4)

- 11).Mohammad Assad, Zahida Perveen, Saira Farman, Beenish Khurshid, <u>Muhammad Ali Hashmi</u>, Khalid Mohammed Khan, Akif Khurshid, "*In Vitro* Screening and MD Simulations of Thiourea Derivatives against SARS-CoV-2 in Association with Multidrug Resistance ABCB1 Transporter", ACS Omega, 2022, 7(51), 47671-47679. (DOI: <u>10.1021/acsomega.2c04671</u>). (I.F. 4.1)
- 12).Amna Ayub, Sehrish Gul, Riffat Ayub, Zeeshana Bibi, <u>Muhammad Ali Hashmi</u>, Ahmed Lakhani, A. Dahshan, Khurshid Ayub, Javed Iqbal, "Porphyrin based Channel for Separation of Proton Isotope: A Density Functional Theory Study", *Journal of Physics and Chemistry of Solids*, 2022, 171, 111032-111038 (DOI: <u>10.1016/j.jpcs.2022.111032</u>). (I.F. 4.0)
- 13).Sania Bibi, Sehrish Sarfaraz, Muhammad Yar, Muhammad Iqbal Zaman, Abdul Niaz, Ayesha Khan, <u>Muhammad Ali Hashmi</u>, Khurshid Ayub, "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*, 2022, 366, 120144-120155 (DOI: j.mollig.2022.120144). (I.F. 6.0)
- 14).Ali Raza Shah, Nasir Rasool, Muhammad Bilal, Adeel Mubarik, <u>Muhammad Ali Hashmi</u>, Muhammad Nadeem Akhtar, Muhammad Imran, Gulraiz Ahmad, Ayesha Siddiqa, Syed Adnan Ali Shah, "Efficient Synthesis of 4-Bromo-N-(1-phenylethyl)benzamide, Arylation by Pd(0) Catalyst, Characterization and DFT Study", *ChemistrySelect*, **2022**, *7*(29), e202200861 (DOI: <u>10.1002/slct.202200861</u>). (I.F. 2.1)
- 15).Adeel Mubarik, Sajad Mehmood, Nasir Rasool, <u>Muhammad Ali Hashmi</u>, Muhammad Ammar, Sadaf Mutahir, Kulsoom Ghulam Ali, Muhammad Bilal, Muhammad Nadeem Akhtar, "Computational Study of Benzothiazole Derivatives for Conformational, Thermodynamic and Spectroscopic Features and Their Potential to Act as Antibacterials", *Crystals*, 2022, 12(7), 912 (DOI: <u>10.3390/cryst12070912</u>). (I.F. 2.7)
- 16). Amna Ayub, Khurshid Ayub, Sehrish Gul, <u>Muhammad Ali Hashmi</u>, Ahmed Lakhani, Saleem Iqbal, Javed Iqbal, "Hetero-Porphyrin based Channel for Separation of Proton Isotope: A Density Functional Theory Study", *Microporous and Mesoporous Materials*, 2022, 339, 111995. (DOI: <u>10.1016/j.micromeso.2022.111995</u>). (I.F. 5.2)
- 17). Adil Khushal, Amara Mumtaz, Wamda Ahmed Shadoul, Syeda Huda Mehdi Zaidi, Hummera Rafique, Abida Munir, Aneela Maalik, Syed Jawad Ali Shah, Ayesha Baig, Wajiha Khawaja, Mariya al-Rashida, <u>Muhammad Ali Hashmi</u>, Jamshed Iqbal, "Synthesis, Carbonic Anhydrase II/IX/XII Inhibition, DFT, and Molecular Docking Studies of Hydrazide-Sulfonamide Hybrids of 4-Methylsalicyl- and Acyl-Substituted Hydrazide", *BioMed Research International*, 2022, 2022, 1-16. (DOI: <u>10.1155/2022/5293349</u>). (I.F. No IF)
- 18). Sehrish Sarfaraz, Muhammad Yar, Muhammad Ans, Mazhar Amjad Gilani, Ralf Ludwig, <u>Muhammad Ali Hashmi</u>, Masroor Hussain, Shabbir Muhammad, Khurshid Ayub, "Computational investigation of a covalent triazine framework (CTF-0) as an efficient electrochemical sensor", *RSC Advances*, 2022, 12, 3909. (DOI: <u>10.1039/d1ra08738i</u>). (I.F. 3.9)
- 19). Iram Gul, Muhammad Yar, Arsalan Ahmed, <u>Muhammad Ali Hashmi</u>, Khurshid Ayub, "Permeability of Boron and Nitrogen Doped Graphene Nanoflakes for Protium/Deuterium Ions", *RSC Advances*, 2022, 12, 3883-3891. (DOI: <u>10.1039/D1RA09398C</u>). (I.F. 3.9)
- 20). Iram Kanwal, Nasir Rasool, Syeda Huda Mehdi Zaidi, Zainul Amiruddin Ahmad, Muhammad Bilal, <u>Muhammad Ali Hashmi</u>, Adeel Mubarik, Gulraiz Ahmad, Syed Adnan Ali Shah, "Synthesis of functionalized thiophene based pyrazole amides via various catalytic approaches: Structural features through Computational applications and Non-linear optical properties", *Molecules*, 2022, 27(2), 360. (DOI: <u>10.3390/molecules27020360</u>). (I.F. 4.6))

Year 2021

21). Yasir Altaf, Sana Ullah, Farhan A. Khan, Aneela Maalik, Syeda Laila Rubab, <u>Muhammad Ali Hashmi*</u>, "Finding new precursors for light harvesting materials: A computational study of the fluorescence

potential of benzanthrone dyes", *ACS Omega*, **2021**, 6, 32334-32341. (DOI: <u>10.1021/acsomega.1c05849</u>). (I.F. 4.1)

- 22). Gulraiz Ahmad, Nasir Rasool, Adeel Mubarik, Ameer Fawad Zahoor, <u>Muhammad Ali Hashmi</u>, Muhammad Zubair, Muhammad Bilal, Mohamed Hussien, Muhammad Saeed Akhtar, Sajjad Haider, "Facile Synthesis of 5-aryl-N-(pyrazin-2-yl)thiophene-2-carboxamides via Suzuki cross-coupling reactions, their electronic and nonlinear optical properties through DFT calculations", *Molecules*, 2021, 26, 7309. (DOI: <u>10.3390/molecules26237309</u>). (I.F. 4.6)
- 23). Komal Rizwan, Nasir Rasool, <u>Muhammad Ali Hashmi</u>, Sadia Noreen, Muhammad Zubair, Mehwish Arshad, Syed Adnan Ali Shah, "Palladium(0) catalyzed synthesis of (E)-4-bromo-N-((3-bromothiophen-2-yl)methylene)-2-methylaniline derivatives via Suzuki cross-coupling reaction: An Exploration of their Non-Linear optical properties, reactivity and structural features", *Molecules*, 2021, 26(18), 5605 (DOI: 10.3390/molecules26185605). (I.F. 4.6)
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