

SHAMSA BIBI
PhD, Post Doc.

PROFILE



DOB : 19 December 1985
Nationality : Pakistan
Material status : Married
Languages : English, Chinese, Urdu, and Punjabi.
Address : Current
Chemistry Department,
University of Agriculture Faisalabad (UAF)
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RESEARCH INTERESTS

Theoretical and Computational analysis of following Materials.

- Organic Photovoltaics (Solar Cells-Donor & Acceptor Materials)
- OLEDs & Florescent Material
- Drug Delivery Material-Nanomaterials
- Dugs Study-Molecular Docking
- NLOs
- Composites and Organometallic Complexes for Pharmaceutical applications
- Schiff-Base metal Complexes analysis

EDUCATION



PhD in Physical/Computational Chemistry, Northeast Normal University, PR China

2010-2014

Dissertation title: Rational Design of the Highly Efficient Sulfur Containing Small Molecular Donor Materials for Organic Photovoltaic Cells.

(1 year Chinese Language 2010-2011)



Master of Science in Chemistry, University of the Punjab, Lahore, Pak Majors: Inorganic / Bio Chemistry

2006-
2008



Bachelor of Science, University of the Punjab, Lahore Pak Majors: Chemistry / Biological Sciences

2004-
2006

WORK



**Postdoctoral
Researcher**

Postdoctoral fellow, State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, PR China

2014-2015



Assistant Professor

Chemistry Department,
University of Agriculture
Faisalabad (UAF)

2015 to May 2024

Associate Professor

May 2024 to date

SCHOLARSHIPS AND AWARDS

- Chinese Government Scholarship (PhD) 2010, Northeast Normal University, PR China
- Postdoctoral Fellowship 2014. State Key Laboratory of Theoretical and Computational Chemistry, Jilin University
- Government Merit scholarship for M.Sc. 2006, Punjab University Lahore, Pakistan.

COMPUTER SKILLS

ChemDraw 12 - CambridgeSoft
OriginPro 8.51- OriginLab
Adobe Photoshop (CS6, Photoshop Touch)
Windows OS, win98-win10
Office Apps - MS Office 1997-2014
Endnote X7
JChemPaint 3.3
ChemSketch 11- ACD Labs

Linux OS - Ubuntu, openSUSE and Fedora

Gaussian 09
Gauss View 5.0.9
Material Studio 7.0
Molekel 5.4.0
PyMolyze 2.0
UltraEdit-32
Mercury 3.0
MATLAB R2014b
Molden 5.2.1
GaussSum 3.0

CALCULATION SKILLS IN COMPUTATIONAL/THEORETICAL CHEMISTRY

- Molecular geometries calculations using Density Functional Theory (DFT) methods.
- Ground state optimization and frequency calculations.
- Molecular orbital calculations.
- Electronic properties calculations.
- Natural transition orbital (NTO) analysis calculations.
- Percentage contribution analysis by calculating total density of states (TDOS) and projected partial density of states (PDOS).
- Simulation of electronic absorption spectra by Time Dependent-DFT (TD-DFT) methods. Reorganization energy calculations in gaseous phase.
- Mobility calculations in the crystalline state structure.
- Generation of the electron density difference map (EDDM) of the transition states to understand the nature of the excited state.
- Potential energy surfaces to predict molecules stability.
- Non-Covalent interaction (NCI) analysis
- IR and NMR calculation analysis

COURSE TAUGHT TO:

Ph.D.
M.Phil.
M.Sc.
Undergraduate
F.Sc Pre-Agriculture

STUDENTS UNDER SUPERVISION

Ph.D. Students (As a Main Supervisor)	=	04 (in progress)
Ph.D. Students (As a Committee Member)	=	02 (in progress)
M.Phil. Students (As a Main Supervisor)	=	158 (completed)
M.Phil. Students (As a Main Supervisor)	=	33 (in progress)
BS/M.Sc. Technical report Students (As a Main Supervisor)	=	51 (Completed)
BS Technical report Students (As a Main Supervisor)	=	49 (Completed)
BS Technical report Students (As a Main Supervisor)	=	11 (in progress)

RESEARCH PROJECTS AND GRANTS

A. Research Projects as PI Awarded

- i. **PI - Start-Up Research Grant Program “Establishment of Computational Chemistry Lab. at UAF” (~ 0.5 million PKR)** by Higher Education Commission Pakistan (**Completed 2015-17**)
- ii. **Awarded International funding** for “**Foreign Research Collaboration Project under “One Road One Belt” project Grant # DL20180036 (~ 37,000 USD) by Jilin University and Ministry of Education of People’s Republic of China**, with institute of Theoretical Chemistry, Jilin University, Changchun, China under, from November 23-30th, 2018-2019 (**completed 2018-19**).
- iii. **International Research collaboration Project by Deanship of Scientific Research, King Khalid University Ministry of Education, Kingdom of Saudia Arabia under project # RGP. 2/272/44 (~ 1.6 million PKR) 2024-25 (Awarded~ continue).**

B. Research Projects as Team Scientist/ Co-PI Equivalent Awarded

1. Punjab Agriculture Research Board (PARB), **Pakistan, Project # 20-419 of 7.794 million PKR by PARB (2021-24 Continue)**
- 2.

RESEARCH PAPERS/ BOOKS PUBLISHED

Abstracts	15
Conferences/Workshops /Trainings	60
PATENTS	
Patents submitted (submitted & under review)	01

Book Chapters

- Haq Nawaz Bhatti and Saima Noreen, **2017**. Principles of Environmental Chemistry. The Caravan Book House Lahore (**Chapter # 02-** Atmospheric Chemistry).
- Haq Nawaz Bhatti and Muhammad Salman, 2017. Applied Chemistry. The Caravan Book House Lahore (**Chapter # 11 &12** Dyes, Paints and Pigments-Paper and Leather Industries.

PUBLICATIONS

2013- to date

Google Scholar Link

<https://scholar.google.com/citations?user=GQzY6L0AAAAJ&hl=en>

Total = 93 (First Author=16 Co-author=27 Corresponding author= 50)

2025

Review Articles = 4

1. Muhammad Zaheer , MuhammadJamshed Latif ^a Sarmed Ali , Saba Jamil , **Shamsa Bibi** ,Shanza Rauf Khan , M. Abdul Rehman “Imobilization of Zero Valent Cobalt and Tin Nanoparticles in Sodium Alginate/Graphitic Carbon Nitride Beads for Efficient Reduction of Organic Pollutants”, **Diamond & Related Materials**, (IF= 4.3) <https://doi.org/10.1016/j.diamond.2025.112320>
2. Iqra Kaifi, Shabbir Muhammad, **Shamsa Bibi***, Shafiq urRehman, Abul Kalam, Aijaz Rasool Chaudhry, Saleh S. Alarfaji, Abdullah G. Al-Sehemi, “Optimizing Core Modifications for High-Performance D-A-D Molecular Systems: A Multi-Faceted Study on NLO Properties, Solvent Effects, Charge Transfer, and Photovoltaic Efficiency”, **Advanced Theory and Simulations (Wiley online)** <https://doi.org/10.1002/adts.202500169>
3. Hafsa & shanza “Biodegradable sodium alginate-based nanohybrid: Tuning reaction conditions for maximum efficiency in wastewater treatment” **International Journal of Biological Macromolecules**, (IF=7.7)
4. Mohammad Y. Alshahrani, Ariha Zaid, Muath Suliman, **Shamsa Bibi***, Shabbir Muhammad, *, Shafiq urRehman “In-silico discovery of efficient second-generation drug derivatives with enhanced antihistamine potency and selectivity”, **Computational Biology and Chemistry**, (I.F=2.6) 8/1/25 <https://doi.org/10.1016/j.compbiochem.2024.108340>
5. **Shamsa Bibi**, Jannat Bibi, Shabbir Muhammad, Shafiq urRehman, Muhammad Adnan, Iqra Kaifi, Aijaz Rasool Chaudhry, “Quantum chemical study of new oxadiazoles as efficient optical and nonlinear optical and photovoltaic materials under gas, PCM and COSMO solvent effects”, **Optics & Laser Technology**, *Volume 182, Part B, April 2025, 112099*(IF=4.6) 28/11 <https://doi.org/10.1016/j.optlastec.2024.112099>
6. HammadAli Khan, Muhammad Irfan, Samreen Gul Khan, **Shamsa Bibi***, Akbar Ali, Iqra Shafiq, Norah Alhokbany, Muhammad Haroon, Humaira Yasmeen Gondal, “Facile Synthesis, Spectroscopic, Electronic and Non-linear Optical Properties of 1,2-4 triazole-based Derivatives: An Experimental and DFT Approach”, **Journal of Molecular Structure** (IF = 4.0 W) 11/11 <https://doi.org/10.1016/j.optlastec.2024.112099>

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7. Shabbir Muhammad, *, Ariha Zaid, **Shamsa Bibi***, Shafiq urRehmana, Mohammad Y. Alshahrani, Santosh Kumar, Muhammad Imran Tousif, Abdullah G. Al-Sehemi, “Piperine analogues as dual inhibitors for antibacterial and antiarthritic properties through impact of ligands optimization, docking and water solvation”, *Journal of Molecular Liquids* (IF=5.3 W), October 29 <https://doi.org/10.1016/j.molliq.2024.126379>
8. Shabbir Muhammad*, Amina Faiz, **Shamsa Bibi***, Shafiq urRehman, Mohammad Y. Alshahrani, Investigation of Dual Inhibition of Antibacterial and Antiarthritic Drug Candidates Using Combined Approach Including Molecular Dynamics, Docking and Quantum Chemical Methods. *Computational Biology and Chemistry* (IF=2.6 X) <https://doi.org/10.1016/j.compbiolchem.2024.108218>
9. Shabbir Muhammad ^a, Adan Ahmad ^b, **Shamsa Bibi***, Shafiq urRehman ^b, AbdullahG. Al-Sehemi ^a, Saleh S. Alarfaji ^a, Aijaz Rasool Chaudhry “Exploring the Impact of Heterocyclic Bridges for Tuning the Amplitudes of Nonlinear Optical Properties under Gas, IEFPCM and COSMO Solvent Models” *Journal of Molecular Liquids* (IF = 5.3 W), sep 24 <https://doi.org/10.1016/j.compbiolchem.2024.108218>
10. **Shamsa Bibi***, ShafiqUr Rehman, Memoona Akram, Rabia Amin, Hafsa Majeed, Shanza Rauf Khan , Saima Younis , Fu-Quan Bai, “Molecular docking and DFT study of antiproliferative ribofuranose nucleoside derivatives targeting EGFR and VEGFR in cancer cells” *Computational Biology and Chemistry* (IF=2.6 X) <https://doi.org/10.1016/j.compbiolchem.2024.108187>
11. Shafiq UrRehman, Mubashra Laraib, Tania Shahzadi, **Shamsa Bibi***, Samreen Gul Khan, Ran Jia, “Designation of efficient diketopyrrolopyrrole based non-fullerene acceptors for OPVs: DFT study” *Material Chemistry and Physics* (IF=4.3 W) <https://doi.org/10.1016/j.matchemphys.2024.129871>
12. Shabbir Muhammad, Alishba Khalid, Shafiq urRehman, **Shamsa Bibi***, Sadia Riaz, Saleh S. Alarfaji, Abdullah G. AlSehemi, Aijaz Rasool Chaudhry, “Designing the electron push-pull chromophores through the joining of triphenylamine and triphenylborane for efficient nonlinear optical and photovoltaic properties”, *Optical Materials*, (IF= 3.8 W) <https://doi.org/10.1016/j.optmat.2024.115253>
13. **Shamsa Bibi**, Aamna Imtiaz, Shabbir Muhammad, Shafiq ur Rehman, Aijaz Rasool Chaudhry, Abdullah G. Al-Sehemi, Bakhet Ahmad Alqurashy, Mazhar Amjad Gilani, “Tailoring the Donor Moieties in TPA-based Organic Dyes for Efficient Photovoltaic, Optical and Nonlinear Optical

- Response Properties”, *Journal: International Journal of Quantum Chemistry* (IF = 2.44 X) <https://doi.org/10.1002/qua.27362>
14. Ammara, sadia Noreen, Sarmad ali, **Shamsa bibi***, saba jamil , Shanza Rauf Khan. CuO/PANI nanocomposite: an efficient catalyst for degradation and reduction of pollutants, *Polymer Bulletin*, (IF= 3.1 X) <https://doi.org/10.1007/s13204-024-03055-w>
 15. Shabbir Muhammad, Sadia Riaz, Shafiq urRehman, **Shamsa Bibi***, Abdullah G. Al-Sehemi, H. Algarni, Aijaz Rasool Chaudhry, “Understanding the Role of Symmetric/Asymmetric Curcuminoids in Designing Efficient Optical, Nonlinear Optical and Photovoltaic Materials”, *Optical and quantum electronics* (IF = 3.0 W) January 2024, vol 56, p.651 <https://doi.org/10.1007/s11082-024-06298>
 16. Hafiz Abdul Mannan, Raziya Nadeem, **Shamsa Bibi***, Tariq Javed, Irum Javed, Arif Nazeer, “Mesoporous activated TiO₂/based biochar synthesized from fish scales as a proficient adsorbent for deracination of heavy metals from industrial efflux” *Journal of Dispersion Science and Technology* (IF 1.9 X) <https://doi.org/10.1080/01932691.2022.2151456>
 17. MuhammadJamshed Latif, Sarmed Ali, Saba Jamil, **Shamsa Bibi***, Touseef Jafar, Ammara Rasheed, Sadia Noreen, Arslan Bashir, Shanza Rauf Khan, “Comparative catalytic reduction and degradation with biodegradable sodium alginate based nanocomposite: Zinc oxide/N-doped carbon nitride/sodium alginate” (IF 7.7 W) <https://doi.org/10.1016/j.ijbiomac.2023.127954>
 18. **Shamsa Bibi** · Sameenal · Shabbir Muhammad² · Shafiq urRehman¹ · Aijaz Rasool Chaudhry³ · Abdullah G. Al-Sehemi¹ · Sajjad Hussain^{4,5} · Shamraiz Hussain Talib⁶Quantum chemical prediction of nonlinear optical and photovoltaic properties and in linear and bent configurations of carbazole/barole derivative, *Arabian journal for science and Engineering*, (IF=2.6 W) <https://doi.org/10.1002/qua.27362>
 19. **Shamsa Bibi**, Iqra Kaifi, Shabbir Muhammad, Shafiq Urrehman, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, Aijaz Rasool Chaudhry, “Quantum Chemical framework for designing high performance ladder shape NLO molecules and study of implicit vs. explicit solvent effect on their NLO properties”, *Journal of Molecular Liquids*, (IF=5.3 W) <https://doi.org/10.1016/j.molliq.2024.125298>
 20. Shabbir Muhammad , Shafiq UrRehman*,Maimoona Zia , **Shamsa Bibi*** , Muhammad Imran Tousif , Aftab Hussain, Tareg M. Belali , Aijaz Rasool Chaudhry , “Use of hybrid molecular simulation techniques for systematic analysis of polyphenols as promising therapeutic agent

against SARS-CoV-2” *Journal of Molecular Structure* (IF= 4.0 W)
<https://doi.org/10.1016/j.molstruc.2024.137744>

21. Shafiq urRehman, Saliha Fatima, Shabbir Muhammad*, **Shamsa Bibi***, Khurram Shahzad Munawar, Abdullah G. Al-Sehemi, Aijaz Rasool Chaudhry, Muhammad Adnan, “Quantum chemical framework for tailoring N/B doped phenalene derivatives to achieve high performance nonlinear optical material”, *Journal of Molecular Graphics and Modelling* (IF= 2.9, X)
<https://doi.org/10.1016/j.jmgm.2024.108723>
22. Shabbir Muhammad, Nimra Zahir, **Shamsa Bibi***, Mohammad Y. Alshahrani, Shafiq-urRehman, Aijaz Rasool Chaudhry, Fatima Sarwar, Muhammad Imran Tousif, “Computational Prediction for Designing Novel Ketonic Derivatives as Potential Inhibitors for Breast Cancer: A trade-off between Drug likeness and Inhibition Potency”, *Computational Biology and Chemistry* (IF =2.6 X) <https://doi.org/10.1016/j.compbiolchem.2024.108020>
23. Rimsha Kanwal, Riyadh R. Al –Araji, Ahmad H. Ibrahim, Dr Muhammad Adnan Iqbal, **Shamsa Bibi***, Adina Zafar, Muhammad Yaseen, Umar Sohail Shoukat and Faisal Jameel, *Photochemical synthesis in inorganic chemistry*, January 2024 *Reviews in Inorganic chemistry* (IF=4.1 X) <https://doi.org/10.1016/B978-0-444-53599-3.10006-X>
24. Muhammad Irfan, Hammad Ali Khan, **Shamsa Bibi***, Gang Wu, Akbar Ali, Samreen Gul Khan, Norah Alhokbany, Faiz Rasool & Ke Chen, “Exploration of Nonlinear Optical Properties of 4-methyl-4H-1,2,4-triazol-3-yl)thio)-N- phenylpropanamide Based Derivatives: Experimental and DFT Approach”, *scientific reports* (IF =3.8 W) Accepted January 2024.
<https://doi.org/10.1038/s41598-024-51788-z>
25. Shafiq-ur Rehman, Hammad Aslam, **Shamsa Bibi***, Nazish Jahan, Muhammad Irfan Majeed, Haq Nawaz, Samreen Gul Khan, Hong-Xing Zhang, “Tuning of End-Groups in Diketopyrrolopyrrole-Based Acceptors Molecules For Organic Photovoltaics”, *Sustainable Chemistry for the Environment* <https://doi.org/10.1016/j.scenv.2024.100068> January 2024
26. Rida Fatima, Javed Iqbal, **Shamsa Bibi***, and Muhammad Yaseen, Exploring acceptor moieties modification in helicene phenylamine-based small molecules for organic and perovskite solar cells, *Journal Energy Technology* (IF=4.15 W), 30th December
<https://doi.org/10.1002/ente.202301019>
27. Shanza Rauf khan, Sajid Ali, Wardah Burhan, Sarmad Ali, Saba Jamil, **Shamsa Bibi***, Naila Bilal, Sabahat Bilal, Jamashed Latif “Comparison effect of gelation on sodium alginate iron oxide nanocomposites for efficient catalytic degradation of organic dyes” *Applied Nanoscience*” <https://doi.org/10.1007/s13204-024-03055-w>

28. Shafiq-ur Rehman *, Ayesha sajjad, **Shamsa Bibi***, Hira Anwar, Saba Jamil, Shanza Rauf Khan, Nadia Munawar, Asim Mansha, Sadia Asim, Hong-Xing Zhang, "A DFT study on removal of Mn and V from wastewater using Chitosan/Graphene oxide composite as adsorbent". 12 December online-*Chemistry of Inorganic Materials* <https://doi.org/10.1016/j.cinorg.2023.100030>
29. Aftab Hussain, Ahmad Irfan, Farah Kanwal, Mohamed Hussien, Mehboob Hassan, Saifedin Y. DaifAllah, Wang Jing, Muhammad Abdul Qayyum, **Shamsa Bibi***, Aijaz Rasool Chaudhry, Jingping Zhang "Exploration of high-performance triptycene-based thermally activated delayed fluorescence materials via structural alteration of donor fragment" online 6th November, *Heliyon* (IF = 3.77 W) <https://doi.org/10.1016/j.heliyon.2023.e21571>
30. Abida Kausar, Sana Ijaz, Mariam Rafaqat, A. Dahshan, Asma Abdul Latif, **Shamsa Bibi***, Nada S. Al-Kadhi, Siham A. Alissa, Arif Nazir, Munawar Iqbal, "Chitosan-cellulose composite for the adsorptive removal of anionic dyes: Experimental and theoretically approach", *Journal of Molecular Liquids* (2023) (IF = 5.3 W) <https://doi.org/10.1016/j.molliq.2023.123347>
31. Saba Jamil^a, Shanza Rauf Khan^a, **Shamsa Bibi***^a, Nazish Jahan^a, Nadia Mushtaq^a, Faisal Rafaqat^a, Rais Ahmad Khan^b, Waqas Amber Gill^c, and Muhammad Ramzan Saeed Ashraf Janjua. Recent advances in synthesis and characterization of iron–nickel bimetallic nanoparticles and their applications as photo-catalyst and fuel additive", *RSC Advances* (IF=3.9) <https://doi.org/10.1039/D3RA04293F>
32. **Shamsa Bibi**, Gulzaib Basharat, Shafiq -ur-Rehman*, Saba Jamil a, Shanza Rauf Khan a, Aftab Hussain b, Ran Jia, "Solvent impact on the photochemical properties of anticancer drug" *Inorganic Chemistry Communications* (IF=4.4W) <https://doi.org/10.1016/j.inoche.2023.111424>
33. Saba Jamil, Shanza Rauf Khan, Sarmed Ali, **Shamsa Bibi***, Rais Ahmad Khan, Waqas Amber Gill, Muhammad Ramzan Saeed Ashraf Janjua." Synthesis of calcium-bismuth layered double hydroxide (LADH) nanoparticles: Applications as photo-catalyst and fuel additive" *Inorganic Chemistry Communications* September 2023 (IF=4.4 X) <https://doi.org/10.1016/j.inoche.2023.111331>
34. **Shamsa Bibi**, Zarina Kousar, Shafiq-ur-Rehman*, Ijaz Ahmad Bhatti, Haq Nawaz Bhatti, Shanza Rauf Khan, Fu Quan Bai, Gohar Farid, "Newly Efficient Designed Benzothiadiazole (A-D- A-D-A topology) based Materials for Organic Photovoltaics: DFT Study", *Materials Today Communications* (July 2023, (IF=3.7 W) <https://doi.org/10.1016/j.mtcomm.2023.106481>

35. Ali Raza, Shanza Rauf Khan, Sarmed Ali, Saba Jamil, **Shamsa Bibi***, Silver/Titanium Nanoparticles Encapsulated Microgel For Catalytic Reduction, *Inorganic Chemistry Communications* (Accepted May 2023 (IF=4.4 X) <https://doi.org/10.1016/j.inoche.2023.110851>
 36. Saba Jamil, Afaaf Rahat Alvi, **Shamsa Bibi***, Nazish Jahan, Syed Ali Raza Naqvi, Shanza Rauf Khan, Khalid Mahmood Zia, Muhammad Ramzan Saeed Ashraf Janjua, “Synthesis, characterization, and applications of cobalt bismuth layered double hydroxide nanoparticles: Physical insights towards a potential material as fuel additive and photocatalyst”, *Journal of Physical Organic Chemistry*, (Accepted Dec 2022 (IF =1.9 X) <https://doi.org/10.1002/poc.4500>
 37. **Shamsa Bibi**, Aamna Saleem, Shafiq-ur-Rehman*, Ijaz Ahmad Bhatti, Muhammad Adnan Iqbal, Raziya Nadeem, Shaid Bashir, Bai Fu Quan, “DFT study of oxidation mechanism of secnidazole as an emerging contaminant; Application as STIs control”, *Journal of Physical Organic Chemistry*, Accepted Dec 2022 (IF = 1.9 X) <https://doi.org/10.1002/poc.4480>
 38. Abida Kousar, Sana Ijaz, Mariam Rafaqat, Dahshan, Asma Abdul Latif, **Shamsa Bibi***, Chitosan- cellulose composite for the absorptive removal of anionic dyes: *Experimental and theoretical approach* <https://doi.org/10.1016/j.molliq.2023.123347>
- 2022**
39. Muhammad Hashaam, Sarmed Ali, Tahreem Khan, Muhammad Salman, Shanza Rauf Khan*, Amjad Islam Aqib, Tean Zaheer, **Shamsa Bibi***, Saba Jamil, Merfat S.Al-Sharif, Samy F. Mahmoud, Wangyuan Yao, “Assembly of Smart Microgels and Hybrid Microgels on Graphene Sheets” for Catalytic Reduction of Nitroarenes”, *Catalysts* (IF = 3.8 W). <https://doi.org/10.3390/catal12101172>
 40. Iqra Shahbaz, Saba Jamil, **Shamsa Bibi***, Shanza Rauf Khan, Muhammad Ramzan Saeed Ashraf Janjua “Recent advances in morphologically controlled synthesis of graphene oxide-based nanocomposite as catalyst and fuel additive”, *Journal of Physical Organic Chemistry*, Accepted Dec 2022 (IF = 1.9 X) <https://doi.org/10.1002/poc.4409>
 41. Saman Naz, Guria bibi, Saba Jamil, Shafiq-urRehman, **Shamsa Bibi***, sarmed Ali, Tehreem Khan, Muhammad Ramdan Saeed Ashraf Janjua, “Preparation of Maganese–doped Tin oxide nanoparticles for catalytic Reduction of Organic dyes” *CPLETT* (IF = 2.8 X) (2022) <https://doi.org/10.1016/j.cplett.2022.139768>.
 42. Fatima Sarwar, Shabbir Muhammad, Shafiq-urRehman, **Shamsa Bibi***, Abdullah G. Al-Sehemi, H. Algarni, Santosh Kumar, “Insighting the systematic impact of shape, size and substitution of heteroatoms in quinoidal oligomers to tune their optoelectronic properties”

<https://link.springer.com/article/10.1007/s11082-022-03724-6>

43. Guria Bibi, Shanza Rauf Khan, Sarmed Ali, Saba Jamil, **Shamsa Bibi***, Hamza Shehroz, Muhammad Ramzan Saeed Ashraf Janjua, Role of capping agent in the synthesis of zinc–cobalt bimetallic nanoparticles and its application as catalyst and fuel additive, *Journal of Applied Nanoscience*, (IF =1.607 2022) <https://link.springer.com/article/10.1007/s13204-022-02468-9>
44. Khurram Shahzad Munawar, Saqib Ali, Abdur Rauf, **Shamsa Bibi***, Muhammad Ashfaq, Muhammad Nawaz Tahir, Shafiq urRehman & Lubna Rasool, “Synthesis, Structural and Computational Analysis, Spectroscopic and Voltammetric Characterization of a Schiff Base” *Journal of the Iranian Chemical Society*, (F = 2.27 X 2022) <https://doi.org/10.1007/s13738-022-02571-2>
45. Shabbir Muhammad, Amna Bibi, Shafiq-urRehman*, **Shamsa Bibi ***, Abdullah G. Al-Sehemi, H. Algarni & Fatima Sarwar “Exploring the quinoidal oligothiophenes to their robust limit for efficient linear and nonlinear optical response properties”, *Chemical Papers* 2022, (IF = 2.1 X); <http://doi.org/10.1007/s11696-022-02167-3>
46. Qurat-Ul-Ain, Sarmed Ali, Saba Jamil, **Shamsa Bibi***, Shanza Rauf Khan, Shafiq-Ur-Rehman, Guria Bibi, Tahreem Khan, Hamza Shehroz, Muhammad Hashaam, Muhammad Ramzan Saeed AshrafJ anjua, “Comparison of catalytic and fuel additive properties of bimetallic nanoparticles and its composite: FeMnO3 and PANI-FeMnO3,” *Materials Science in Semiconductor Processing* 2021. (IF = 4.2 W) <https://doi.org/10.1016/j.mssp.2022.106630>
47. Muhammad Waheed Mushtaq, Shifa Tariq, Aisha Hameed, Shahid Bashir, **Shamsa Bibi***, Naveed Aslam Dogar, Aisha Batool and Saira Ishaq, “Spectrophotometric determination of vitamin C in underground vegetables and kinetic modelling to probe the effect of temperature and pH on degradation of vitamin C”, *Pakistan Journal of Botany* (2022) (I.F=1.2 X) [http://dx.doi.org/10.30848/PJB2022-5\(12\)](http://dx.doi.org/10.30848/PJB2022-5(12)).
48. Asim Mansha, Syeda Anam Asad, Sadia Asim, **Shamsa Bibi***, Shafiq-Ur- Rehman, Alina Shahzad, “Review of recent advancements in fluorescent chemosensor for ion detection via coumarin derivatives”, **Chemical Papers** (IF=2.15 X) <https://doi.org/10.1007/s11696-022-02092-5>
49. **Shamsa Bibi**, Shafiq Ur-rehman,* Laryeb Khalid, Ijaz Ahmad Bhatti, Haq Nawaz Bhatti, Javed Iqbal, Fu Quan Bai and Hong-Xing Zhang, “Investigation of adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug delivery carrier; DFT Study”. *RSC Advances* (IF = 3.9 W) 2021 <https://doi.org/10.1039/D1RA09319C>

50. Aqsa Mukhtar, Asim Mansha, Sadia Asim, Alina Shahzad, **Shamsa Bibi***, “Excited State Complexes of Coumarin Derivatives”. *Journal of Fluorescence* (2021). (IF 2.6 W) <https://doi.org/10.1007/s10895-021-02807-z>
51. Shabbir Muhammad, Shafiqur Rehman*, Fatima Sarwar, **Shamsa Bibi***, Raziya Nadeem, Muhammad Waheed Mushtaq, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, Sajjad Hussain, “Insighting the functionally modified C60 fullerenes as an efficient nonlinear optical materials: A quantum chemical study” *Materials Science in Semiconductor Processing* 2021. (IF = 4.2 W) <https://doi.org/10.1016/j.mssp.2021.106421>
52. Shafiq UrRehman *, Makhvela Anwer, **Shamsa BiBi***, Saba Jamil, Muhammad Yasin, Shanza Rauf Khan, Raziya Nadeem, Sarmed Ali, Ran Jia, “DFT analysis of different substitutions on optoelectronic properties of carbazole-based small acceptor materials for Organic Photovoltaics”. *Materials Science in Semiconductor Processing* 2021 (IF = 4.2 W). <https://doi.org/10.1016/j.mssp.2021.106381>

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53. Aamna Ashfaq, Razyia Nadeem, **Shamsa Bibi***, Umer Rashid, Asif Hanif ,Nazish Jahan ,Zeeshan Ashfaq, Zubair Ahmed, Muhammad Adil, Maleeha Naz, “Efficient Adsorption of Lead Ions from Synthetic Wastewater Using Agrowaste-Based Mixed Biomass (Potato Peels and Banana Peels)” *Journal of Water* (MDPI) (2021) (IF = 3.00). <https://www.mdpi.com/2073-4441/13/23/3344>
54. Amna Bibi, Shabbir Muhammad, Shafiq UrRehman, **Shamsa Bibi***, Shahid Bashir, Khurshid Ayub, Muhammad Adnan, and Muhammad Khalid, “Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties”. *ACS Omega* (2021) (IF =4.1 W) <https://doi.org/10.1021/acsomega.1c03218>
55. UmerYaqoob, Sidra Rafiq, Shafiq-ur Rehman, **Shamsa Bibi***, Javed Iqbal “Designing and Comparative Analysis of 3D Subphthalocyanines Based Non-Fullerene Acceptor Molecules as An Efficient Material for Organic Solar Cells”. *Optik* (2021). (IF =2.187 W) <https://doi.org/10.1016/j.ijleo.2021.167845>
56. Sarmad Ali, Sayyed Junaid Ul Hassan, Saba Jamil, **Shamsa Bibi***, Muhammad Usman Shah, Amjad Islam, Aqib, Tean Zaheer, Shanza Rauf Khan, Muhammad Ramzan Saeed Ashraf Janjua, “Zirconium Nanoparticles-Poly (N-isopropylacrylamidemethacrylic acid) Hybrid Microgels

- Decorated Graphene Sheets for Catalytic Reduction of Organic Pollutants”. Journal of *Chemical Physics letters*, (2021). (IF=2.8 X) <https://doi.org/10.1016/j.cplett.2021.138915>
57. **Shamsa Bibi**, Shafiq-Ur-rehman, Laryeb Khalid, Muhammad Yaseen, Abdul Quyyam Khan, Ran Jia. “Metal Doped Fullerene Complexes as Promising Drug Delivery Materials against COVID-19”. Journal of *Chemical Papers*”(2021).(IF=2.1 X) <https://doi.org/10.1007/s11696-021-01815-4>
 58. **Shamsa Bibi**, Faiza Farooq, Shafiq-ur-Rehman, Fu-Quan Bai, Hong-Xing Zhang, “DFT and TD-DFT studies of Phenothiazine Based Derivatives as Fluorescent Materials for Semiconductor Applications”. *Materials Science in Semiconductor Processing* 2021. (IF =4.2 W). <https://doi.org/10.1016/j.mssp.2021.106036>
 59. Shazia Perveen, R. Nadeem, Munawar Iqbal, **Shamsa Bibi***, Rohama Gill, Rashid Saeed, Saima Noreen, Kalsoom Akhtar, Tariq Mehmood Ansari, Nada Alfryyan.“Graphene oxide and Fe₃O₄ composite synthesis, characterization and adsorption efficiency evaluation for NO₃⁻ and PO₄³⁻ ions in aqueous medium”. *Journal of Molecular Liquids* (2021). (IF = 5.3 W). <https://doi.org/10.1016/j.molliq.2021.116746>
 60. Dong-ChunYang, Yong-BoTan, Roberts I.Eglitis, **Shamsa Bibi***, Ran Jia, Hong-XingZhang. “Dipoles in 4,12,4-graphyne”. *Applied Surface Science*, (2021). 545: p. 148991. (IF =6.3 W) <https://doi.org/10.1016/j.apsusc.2021.148991>
 61. Maimoona Zia, Shabbir Muhammad, Shafiq-urRehman, **Shamsa Bibi***, Sumra Wajid Abbasi, Abdullah G Al-Sehemi, Aijaz Rasool Chaudhary, Fu Quan Bai. “Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies”. *Bioorganic & Medicinal Chemistry Letters* (2021). Vol 43. PMID: 33940136. PMC8087859. (IF = 2.5) <https://doi.org/10.1016/j.bmcl.2021.128079>
 62. Abida Kausar, Ramsha Shahzad, Sadia Asim, **Shamsa Bibi***, Jibran Iqbal, Nawshad Muhammad, Mika Sillanpa, Israaf UdDini. “Experimental and theoretical studies of Rhodamine B direct dye sorption onto clay-cellulose composite”. *Journal of Molecular Liquids*, (2021). 328:p. 115165. (IF=5.3 W) <https://doi.org/10.1016/j.molliq.2020.115165>
 63. Shafiq-ur-Rehman, Shaista Ghafoor, **Shamsa Bibi***, Abida Kausar, Shaukat Ali, Sadia Asim, Asim Mansha, Syeda Aaliya Shehzadi & Ran Jia. “DFT and TD-DFT Studies of Non-Fullerene Organometallic Based Acceptors for Organic Photovoltaics”. *Journal of Inorganic and Organometallic Polymers and Materials* (2021). (IF=3.9 W) <https://doi.org/10.1007/s10904-020-01833-x>

64. **Shamsa Bibi**, Mehwish Khan, Shafiq ur-Rehman, Muhammad Yaseen, Shabbir Muhammad, Raziya Nadeem, Nazish Jahan, Saima Noreen, Misbah. Investigation analysis of optoelectronic and structural properties of cis- and trans-structures of azo dyes: density functional theory study. *Journal of Physical Organic Chemistry*, (2021). (IF =1.9 X) <https://doi.org/10.1002/poc.4183>
65. Adeena Asif, Rana Yasir Nadeem, Muhammad Adnan Iqbal, **Shamsa Bibi***, Muhammad Irfan. “Organometallic complexes of neodymium: an overview of synthetic methodologies based on coordinating elements”. *Reviews in Inorganic Chemistry*, (2021). (IF =4.1 X) <https://doi.org/10.1515/revic-2020-0019>
66. Muhammad Shoaib, Shaffiq ur- Rehman, **Shamsa Bibi***, Inam Ullah, Saba Jamil, Javed Iqbal, Asma Alam, Ushna Saeed, Fu Quan Bai. “Theoretical Investigation of Perylene Diimide derivatives as Acceptors to Match with Benzodithiophene based Donors for Organic Photovoltaic Devices”. *Zeitschrift für Physikalische Chemie*, (2019). (IF=2.408 X) <https://doi.org/10.1515/zpch2019-1451>
67. Sana Akram, Azra Quraishi, Nadia Zulficar, Madiha Akbar, **Shamsa Bibi***, “Investigating the use of diketopyrrolopyrrole (DPP) based highly conjugated small molecules in organic solar cells” *Scientific Inquiry and Review* (Y category) <https://doi.org/10.32350/sir.51.02>

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69. Muhammad Sohail, Muhammad Zeshan Ashraf, Raziya Nadeem, **Shamsa Bibi***, Rabia Rehman, Muhammad Adnan Iqbal. *Techniques in the synthesis of organometallic compounds of tungsten. Reviews in Inorganic Chemistry*, (2020). 40(1), 1-45. (IF=4.1 X) <https://doi.org/10.1515/revic-2019-0013>
70. Shanza Rauf Khan, Maria Batool, Saba Jamil, **Shamsa Bibi***, Sobia Abid, Muhammad Ramzan Saeed Ashraf Janjua. Synthesis and characterization of Mg–Zn bimetallic nanoparticles: Selective hydrogenation of p-nitrophenol, degradation of reactive carbon black 5 and fuel additive. *Journal of Inorganic and Organometallic Polymers and Materials*, (2020). 30(2), 438-450. (IF=3.9 W) <https://doi.org/10.1007/s10904-019-01202-3>
71. Shanza Rauf Khan, Saba Jamil, **Shamsa Bibi***, Sarmed Ali, Tanzila Habib, Muhammad Ramzan Saeed, Ashraf Janjua. “A Versatile Material: Perovskite Bismuth Ferrite Microparticles as a Potential Catalyst for Enhancing Fuel Efficiency and Degradation of Various Organic

- Dyes". *Journal of Inorganic and Organometallic Polymers and Materials*. 2020, (IF = 3.9 W). <https://doi.org/10.1007/S10904-020-01520-X>
72. Shafiq UrRehman, Asma Alam, **Shamsa Bibi***, Sana Sadaf, Shanza Rauf Khan, Muhammad Shoaib, Abdul Qayyum Khan, Mehwish Khan, Waheed UrRehman. The effect of different aromatic conjugated bridges on optoelectronic properties of diketopyrrolopyrrole-based donor materials for organic photovoltaics. *Journal of Molecular Modeling*, (2020). 26(6), 154-154. (IF=2.2 X). <https://doi.org/10.1007/s00894-020-4341-8>
 73. Muhammad Yaseen, Amna Ashfaq, Anum Akhtar, Rida Asghar, Hina Ambreen, Mehwish Khalid Butt, Saima Noreen, Shafiq Ur Rehman, **Shamsa Bibi***, Shahid M Ramay. "Investigation of LaAlO₃ perovskite compound for optoelectronic and thermoelectric devices under pressure". *Materials Research Express*, (2020). 7(1), 015907. (IF=1.8 X) <https://doi.org/10.1088/2053-1591/ab6110>
 74. Muhammad Yaseen, Muhammad Dilawar, Hina Ambreen, **Shamsa Bibi***, Shafi Ur Rehman, Umair Shahid, Mehwish Khaid Butt, Abdul Ghaffar, Adil Murtaza. "Electronic, optical and magnetic properties of low concentration Ni-doped CdSe by first principle method". *Bulletin of Materials Science*, (2020). 43(1). (IF=1.9) <https://doi.org/10.1007/s12034-020-2078-8>
 75. Muhammad Yaseen, Hina Ambreen, Abu Sufyan, Mehwish Khlid Butt, M. K., Shafiq UrRehman, Javed Iqbal, Misbah, **Shamsa Bibi***, Adil Murtaza, Shahid M.Ramay. Optical and magnetic properties of manganese doped zinc sulphide: density functional theory approach. *Ferroelectrics*, (2020). 557(1), 112-122. (IF=0.620 Y) <https://doi.org/10.1080/00150193.2020.1713356>

2019

76. Munazza Naseem, Sana Sadaf, **Shamsa Bibi***, Habib-ur- Rehman, Mehmood-u-Hassan, Saira Aziz, Inam Ullah. "Evaluation of a NIAB Gold castor variety for biodiesel production and bio-pesticide". *Industrial Crops and Products*, (2019). 130, 634-641. (IF=5.645 W) <https://doi.org/10.1016/j.indcrop.2019.01.022>
77. Waheed ur Rehman & Guiyun, Jiang & Yongqin, Wang & Iqbal, Muhammad, Shafiq ur rehman, **Shamsa Bibi***, Elahi, Hassan. A New Type of Aerostatic Thrust Bearing Controlled by High-speed Pneumatic Valve and a Novel Pressure Transducer. *International Journal of Automotive and Mechanical Engineering*, (2020). 16(4), 7430-7446. (IF=1.928 X). <https://doi.org/10.15282/ijame.16.4.2019.16.0550>
78. Waheed Ur Rehman, Jiang Guiyun, uo YuanXin, Wang Yongqin, Nadeem Iqbal, Shafiq UrRehman, **Shamsa Bibi***. "Linear extended state observer-based control of active lubrication

for active hydrostatic journal bearing by monitoring bearing clearance”. *Industrial Lubrication and Tribology*, (2019). (IF=1.5 X) <https://doi.org/10.1108/ILT-09-2017-0263>

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80. Ushna Saeed, Dr. **Shmasa Bibi***, Dr. Shafiq Ur-Rehman, Shanza Rauf khan, Muhammad Shoaib, Dr. Muhammad Adnan Iqbal, Dr. Faisal Nawaz, Dr. Ran Jia. “Designation and Match of Non-Fullerene Acceptors with X-Shaped Donors toward Organic Solar Cells”. *ChemistrySelect*, (2019). 4(13), 3654-3664. (I.F=2.109 X) <https://doi.org/10.1002/SLCT.201803821>
81. **Shamsa Bibi**, Shafiq-Ur-Rehman, Ran Jia, Hong-Xing Zhang, Fu-Quan Bai. “Effect of different topological structures (D- π -D and D- π -A- π -D) on the optoelectronic properties of benzo [2, 1-B: 3, 4-B'] dithiophene based donor molecules toward organic solar cells”. *Solar Energy*, (2019). 186, 311-322. (IF=6.00 W). <https://doi.org/10.1016/j.solener.2019.04.043>
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83. Ahmad Waqas, **Shamsa Bibi***, Shafiq-ur-Rehman, Sufian Afzal, Muhammad Yaseen, Muhammad Shoaib, Ushna Saeed, Wang Da Ming. “Substitutional effect of different bridging groups on optical and charge transfer properties of small bipolar molecules for OLEDs”. *Journal of Physical Organic Chemistry*, (2019). 32(11), e4000. (IF=1.9 X) <https://doi.org/10.1002/poc.4000>

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84. Waheed Ur Rehman, Jiang Guiyun, Nadeem Iqbal, Luo Yuanxin, Wang Yongqin, Shafiq Ur Rehman, **Shamsa Bibi***, Farrukh Saleem, Irfan Azhar, Muhammad Shoaib. “Intelligent Servo Feedback Control for Hydrostatic Journal Bearing”. In: Li K., Fei M., Du D., Yang Z., Yang D. (eds) *Intelligent Computing and Internet of Things. ICSEE 2018, IMIOT 2018. Communications in Computer and Information Science*, vol 952, p364-364. (IF=0.48). https://link.springer.com/chapter/10.1007/978-981-13-2384-3_33

2017

85. Muhammad Adnan, Javed Iqbal, **Shamsa Bibi***, Riaz Hussain, Muhammad Nadeem Akhtar, Muhammad Abid Rashid, Bertil Eliasson, Khurshid Ayub. “Fine Tuning the Optoelectronic

Properties of Triphenylamine Based Donor Molecules for Organic Solar Cells”. *Zeitschrift für Physikalische Chemie*, (2017). 231(6), 1127. (IF=2.408 X).
<https://doi.org/10.1515/zpch-2016-0790>

86. Peng Fu, Jing Wang, Ran Jia, **Shamsa Bibi***, Roberts I. Eglitis, Hong-Xing Zhang. “Theoretical study on hydrogen storage capacity of expanded h-BN systems”. *Computational Materials Science*, (2017). 139, 335-340. (IF=3.1W) <https://doi.org/10.1016/j.commatsci.2017.08.015>
87. Zeenat Zara, Dr. Javed Iqbal, **Dr. Shamsa Bibi***, Dr. Sana Sadaf, Dr. Berti Eliasson “Designing Benzodithiophene-Based Donor Materials with Favorable Photovoltaic Parameters for Bulk Heterojunction Organic Solar Cells”. *ChemistrySelect*, (2017). 2(20), 5628-5639. (IF=2.109 X) <https://doi.org/10.1002/slct.201701008>
88. Zhi-Xiang Zhang, Wei Wei, Fu-Quan Bai, **Shamsa Bibi***, Hong-Xing Zhang. “The phosphorescence properties of a series of diarylethene-containing platinum complexes: the effect of ligand photoisomerization”. *Organic Chemistry Frontiers*, (2017). 4(11), 2191-2201. (IF=4.6 W) <https://doi.org/10.1039/C7QO00476A>

2016

89. **Shamsa Bibi**, Jingping Zhang. “Theoretical studies to investigate the effect of different cores and two different topologies on the optical and charge transfer properties of donor materials for organic solar cells”. *New Journal of Chemistry*, (2016). 40(4), 3693-3704. (IF=2.7 W) <https://doi.org/10.1039/C5NJ02412A>

2015

90. Li Hao, Fu-Quan Bai, Chui-Peng Kong, **Shamsa Bibi***, Hong-Xing Zhang. “Theoretical studies of heteroatom-doping in TiO₂ to enhance the electron injection in dye-sensitized solar cells”. *RSC advances*, (2015). 5(97), 79868-79873. (IF=3.9W) <https://doi.org/10.1039/C5RA15282H>
91. **Shamsa Bibi**, Jingping Zhang. “The ratio and topology effects of benzodithiophene donor–benzooxadiazole acceptor fragments on the optoelectronic properties of donor molecules toward solar cell materials”. *Physical Chemistry Chemical Physics*, (2015). 17(12), 7986-7999. (IF=3.676 (W) <https://doi.org/10.1039/C4CP05814C>

2013

92. **Shamsa Bibi**, Ping Li, Jingping Zhang. “X-Shaped donor molecules based on benzo [2, 1-b: 3, 4-b'] dithiophene as organic solar cell materials with PDIs as acceptors”. *Journal of Materials Chemistry A*, (IF=10.7 W) <https://doi.org/10.1039/C3TA12421E>

CONFRENESS PAPER

93. Waheed Ur Rehman, Luo Yuanxin, Jiang Guiyun, Wang Yongqin, Shafiq Ur Rehman, **Shamsa Bibi***, Nadeem Iqbal, Mansoor Ali Zaheer, Irfan Azhar, Yang Xiaogao, (2017). "Control of oil film thickness for hydrostatic journal bearing using PID disturbance rejection controller," 2017 *IEEE 3rd Information Technology and Mechatronics Engineering Conference (ITOEC)*, 2017, pp. 543-547, (IF=3.557) <http://doi.org/10.1109/ITOEC.2017.8122355>

ADDITIONAL ADMINISTRATIVE SERVICES (03)

- i. Acting As **"Deputy Hall Warden (Female) "PARS, UAF** from 01/09/2023 to date).
- ii. Acting as **Superintendent of Arnic Hall, PARS** from 26/10/2022 to date.
- iii. **Co-Tutor** of Qasim-3, at UAF Community College, PARS from 26/10/2022 to date.

ADMINISTRATIVE SERVICES ASSIGNED BY DEAN/ DIRECTOR/ CHAIRMAN ON ANNUAL BASIS

- i. Acting as **Female Advisor for undergraduate students** at department of Chemistry from 01/09/2022 to date).
- ii. Acting as **Departmental Website Focal Person** for department of Chemistry from June 2023 to date
- iii. Acting as **CO-Organizer of Chemical Society, at department of Chemistry** September 2022 to date.
- iv. Acting as member of **"Course Review and Course File Committee"** of Chemistry Department from 01/07/2022 to date).
- v. Acted as **Manager for Squash Female Team, Faculty of Sciences, UAF Sports League** 2021-2022.
- vi. Acted as **Coach for Cricket Female Team, Faculty of Sciences, UAF Sports League** 2023-24.
- vii. Acted as Committee member of team for "Chinese Delegation Visit at UAF about QINCHAIINSTITUTE OF SALT LAKES INEST ABLISHING A RESEARCH CENTER OF HIMALAYAN ROCK SALT IN PAKISTAN".
- viii. Acted as, **In charge of the 'Female Students Matters Committee'** at UAF Community College PARS 2016-2018.

COMMUNITY SERVICES

- a) **Performed Election Duty As "Presiding Officer"** during General Elections of Pakistan, 2018.
- b) **Performed Election Duty As "Presiding Officer"** during General Elections of Pakistan, 8th February 2024.

- c) *Duty performed in wheat campaign* by University of Agriculture Faisalabad by collaboration with ‘*Punjab Government Agriculture department extension*’ from 12 -20th November 2021.

ACTING AS REVIEWER

As journal Editor/referee

1. Acting as “Journal CO-Guest Editor” for journal “Frontiers in Chemistry” research topic entitled as “*Molecular System Theoretical Calculations for Organic Electronics*” year 2023 to date.
2. Acting As a Reviewer for “Advances in Science, Technology and Engineering Systems Journal (ASTESJ)” from Oct 2017.
3. Acting as Referee for “IOP Science” from April 5th, 2019.
4. Acting as a Reviewer for “World Journal of Surgical Oncology” from June 2019 to date.
5. Acting as a Reviewer for “*Fibers and Polymers*” from 2021 to date.
6. Acting as a Reviewer for “*Polymer for Advanced technologies by Wiley*” from 2021 to date.
7. Reviewer for Journal “*Results in Chemistry*” (from 28 July 2022-Present).
8. Acting as a Reviewer for “Computers in Biology and Medicine” by from March 2024 to date.

M. Phil Thesis evaluation (Acting as External Examiner)

2024

- i. As External Examiner of student names” Amina Parveen” ID no. MSF2204539, Session 2022-2024 of M.Phil. entitled as” Surface -enhanced Raman spectroscopy for characterization of residue and filtrate portions of blood serum samples of breast cancer.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (June 2024).
- ii. As External Examiner of student names” Rahila” ID no. MSF2204537, Session 2022-2024 of M.Phil. entitled as” NMR Cyclic Volumetry and Dynamic Light Scattering Study (DLS) Of Microemulsion System.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (July 2024).
- iii. As External Examiner of student names” Muhammad Ahsan Jawad” Roll no. 2221201, Session 2022-2024 of M.Phil. entitled as” Synthesis characterization and biological evaluation of Naphthalene-1-amine based ligands and their metal complexes.” at Department of Chemistry, University of Education Lahore, Faisalabad Campus, (October 2024).

2022

- iv. As External Examiner of student names” Fazeelat” registration no. 2016-GCWUF-2665, Session 2020-2022 of M.Phil. entitled as” Development of oleo gels: promotion of healthy

skincare products” from wastepaper: experimental and theoretical studies.” at Department of Chemistry, GCW University, and Faisalabad (viva held on 22nd November 2022).

- v. As External Examiner of student names” Kinza” registration no. 2017-GCWUF-0945, Session 2019-2021 of M.Phil. entitled as” Strengthening adsorption process for water contaminated by pharmaceutical compounds using cellulose derived from waste paper: experimental and theoretical studies.” at Department of Chemistry, GCW University, and Faisalabad (January 2022).

2021

- vi. As External Examiner of student names” Rabia Tabassum” Roll No. 509, Session 2019-2021 of M.Phil. entitled as” Synthesis and Characterization of Lead-Free Halides Double Perovskite Materials” at Department of Chemistry, GC University, Faisalabad. (November 2021).
- vii. As External Examiner of student names” Tayyba Shoukat” Roll No. 601, Session 2019-2021 of M.Phil. entitled as” Facile Synthetic Routes of Graphene Quantum Dots from Indigenous Coal And Their Characterization” at Department of Chemistry, GC University, Faisalabad. (December 2021).
- viii. As External Examiner of student names” Saba Yaqoob” Roll No. 613, Session 2019-2021 of M.Phil. entitled as” Synthesis, Antibacterial and Insilico Modeling of Novel Oxadiazole Derivatives As Potential Therapeutics” at Department of Chemistry, GC University, Faisalabad. (December 2021).

2021

- ix. As External Examiner of student names” Sundus Aziz” Roll No. 2013-GCWUF-0779, Session 2018-2020 of M.Phil. at Department of Chemistry, GCW University, Faisalabad.
- x. As External Examiner of student names” Ajmal Shezad” Roll No. 395333, Session 2018-2020 of M.Phil. at Department of Chemistry, GC University, Faisalabad.
- xi. As External Examiner of student names” Farwa Khalid” Roll No. 2014-GCWUF-1931, Session 2018-2020 of M.Phil. at Department of Chemistry, GCW University, Faisalabad.
- xii. As External Examiner of student names” Zainib Razzaq” Roll No. 614, Session 2019-2021 of M.Phil. at Department of Chemistry, GC University, Faisalabad.

2019

- xiii. As External Examiner of student names” Mr. Rizwan Ali Roll No. 26401, Session 2017-2019 of M.Phil. at Department of Chemistry, GC University, Faisalabad.

PhD Comprehensive Examiner

- i. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Unha Tahir, Reg No. 2016-ag-3101” held on 10/11/2022 at 2: 30 pm, in the Video Conference Room (DFS) UAF.
- ii. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Arifa Murtaza, Reg No. 2015-ag-1035” held on 24/11/2022 at 2: 30 pm, in the Video Conference Room (DFS) UAF.
- iii. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Miss Arooj Fatima, Reg No. 2018-ag-4031” held on 06/11/2022 at 11 am, in the Video Conference Room (DFS) UAF.
- iv. Acted as member of Board of Examiner of PhD Comprehensive Examination for PhD student Named “Mr. Ghulam Mustafa, Reg No. 2015-ag-3586” held on 16/07/2021 at 2pm, in the Video Conference Room DLC-I UAF.

EVENTS ORGANIZED AS ORGANIZING SECRETARY

1. Organized Two days 1st International Symposium on “*FRONTIERS IN COMPUTATIONAL CHEMISTRY (FCC-2022)*” at Department of Chemistry, University of Agriculture, Faisalabad, July 4-5th, 2022.
2. ***Organized 1st International seminar on "DFT: A Multidimensional Exploration" (DFT-ME 2024)*** on July 23rd, 2024, at the Science Block Lecture Theatre, UAF.

EVENTS ACTED AS ORGANIZING COMMITTEE MEMBER

3. **Acted as Organizing committee member of** “poster management/scientific/registration committee” International Conference on Functional Materials and Emerging Technologies (ICFMET-2024)” at Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
4. **Acted as Organizing committee member** publication in ‘two-day International Symposium’ on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.
5. **Acted as Organizing committee member** in “One Day Nano-Tech Meeting on Wastewater Treatment” at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3rd, 2019.
6. **Acted as Organizing committee member** in ‘National Workshop on Technical and Patent Writing’ by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, January 28th, 2017.

TRAINING

1. Participation in '**National training Workshop on X-ray Crystallography**' by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, November 7-December 2, 2016.
2. Participation in a **two-day training workshop "Statistical Methods for Researchers using R"** by Department of Mathematics and Statistics, University of Agriculture Faisalabad-Pakistan, August 09-10, 2017. University Faisalabad, Pakistan, May 4 - 5, 2017.
3. Participation in '**National training Workshop on Advanced Spectroscopic techniques for Characterization of organic Compounds**' by Department of Chemistry and Central Hi-Tech Laboratory, University of Agriculture Faisalabad-Pakistan, August 15-16, 2017.
4. Participation in **international training on "Recent Advances in Computational Chemistry" at Institute of Theoretical Chemistry, Jilin University Changchun 130023, China**, Under "One Road One Belt Project" (Grant # DL20180036) from State Administration of Foreign Expert Affairs of China Aug. 08-21, 2019.
5. **Participated in two days Election Training of presiding officer** at Government Crescent School, Faisalabad, arranged by **Election Commission of Pakistan**, in May 2023.

Acted as member of Tender Purchase committee

- a. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as "Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops".
- b. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as "Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops", held on February 3rd, 2022.
- c. *Acted as member of Tender Committee* for equipment purchase for a PARB project# 20-419 entitled as "Preparation and Commercialization of coated micronutrients and control release for improving yield and quality of crops", held on February 9th, 2022.

ORAL /POSTER PRESENTATIONS

6. **Abstract publication and Oral Presentation** in '**7th International Conference "Environmentally Sustainable Development", ESDev-2017**' at **CIIT Abbottabad, Pakistan**, August 26-28, 2017.
7. **Oral presentation** in "First International Conference on Intelligent Manufacturing and Internet of Things and 5th International Conference on Computing for Sustainable Energy and Environment, **IMIOT and ICSEE 2018, Chongqing, China, September 21-23, 2018**.
8. **Oral Presentation and Abstract publication** in '**2nd international conference Chemistry Conference of Biochemistry, Biotechnology and Biomaterials, 2018**' at Department of Biochemistry, University of Agriculture, Faisalabad, Pakistan, December 09-011, 2018.

9. **Poster Presentation and Abstract** publication in ‘two day International Symposium’ on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.
10. **Poster presentation and abstract** publication in “2nd International Conference on Recent Advances in Chemical Sciences, ICRAC 2019” at Department of Chemistry, GC University Lahore, Mar 20-22, 2019.
11. **Oral Presentation and Abstract** publication in ‘International Chemistry Conference forefronts of Chemistry, Celebrating the Periodic Table Year’, at Institute of Chemical Sciences BZU Multan, Mar 27-29, 2019.
12. **Oral Presentation and Abstract** publication in ‘The Seventeenth International Symposium on Electroanalytical Chemistry & The Third International Meeting on Electrogenenerated Chemiluminescence (17th ISEAC & 3rd ECL)’, at Changchun Institute of Applied Chemistry Chinese Academy of Sciences 5625 Renmin Street, Changchun, Jilin 130022, China, Aug 22-25, 2019.
13. **Invited speaker in “Multidisciplinary** Approach towards Computational Chemistry”, at GCWUF, Faisalabad, Sep 25-26, 2019.
14. **Oral presentation as Invited speaker** in “2nd International Conference on Advances in Theoretical and Applied Physics”, at GCWUF, Faisalabad, Mar 2-3, 2020.
15. **Oral presentation as Guest speaker** in “International Conference on Advances in Experimental and Theoretical Physics”, at UAF, Faisalabad, Mar 4-5, 2020.
16. **Oral Presentation** in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
17. **Poster Presentation** in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
18. **Oral Presentation** in Two Day 5th National and 1st International Symposium on Writing Science and Leveraging Scientific Research”, organized by Department of Chemistry, University of Agriculture, Faisalabad, March 02-03, 2022.
19. **Oral Presentation** in workshop on “Helping People to Develop safe and Sustainable Water for Use”, organized by Department of Chemistry, University of Agriculture, Faisalabad, December 23rd, 2022.
20. **Oral Presentation** in online webinar on “Molecular Docking an DFT studies for Drugs Development” organized by Department of Chemistry, University of Agriculture Faisalabad Pakistan, on 25th January.

21. **Invited Talk** in Three Days 4th International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, December 4-6th, 2024.
22. **Invited Talk** in Three Days International Conference on “Natural Products: Biological and pharmaceutical Applications”, organized by Department of Chemistry, Government College Women University, Faisalabad, December 18-20th, 2024.
23. **Invited Talk** as Keynote speaker in One day International Symposium on “1st International Symposium on Computational Chemistry/Machine Learning”, organized by Department of Chemistry, COMSATS University Islamabad, Lahore Campus, April 16, 2025.

PARTICIPATION IN CONFERENCES/WORKSHOPS/ REFRESHER COURSES & TRAININGS

24. **18th National Chemistry Conference, Institute of Chemistry, University of the Punjab, Lahore**, Chemical Society of Pakistan, Feb. 2008.
25. **International Conference** on Computational Chemistry and Biology (ICCCB) November 2012 Shenzhen, China.
26. **International Conference** on Theoretical and High Performance Computational Chemistry 2012 , Nanjing , China
27. The Seventh International Conference on Theoretical Chemistry Molecular Modeling and Life Sciences as well as Academic Intercommunion on the Platform for Scientific Computation and Simulation Software (7th ICTCLS), Beijing, China, July 2013.
28. The **12th National Conference** of Quantum Chemistry (NCQC), Taiyuan, China, June 2014.
29. Participation in ‘**National Grant Writing Workshop**’ by US-Pakistan center for Advance Studies in Agriculture and Food Security (USPCAS-AFS) at UAF, April 6-7, 2016.
30. Participation in **National workshop** on “Organic Food and Health: Avenues of Innovation and entrepreneurship’ University of Management and technology, Lahore, Pakistan by Pakistan Council for Science and Technology (PCST), August 29, 2016.
31. Participation in ‘**International Conference** on Energy for Environmental and Economic Sustainability (ICEEES2016)’ Lahore, Pakistan October 20 - 23, 2016.
32. Participation in ‘27th National and **International Chemistry Conference** at Department of Chemistry’, University of Malakand, Khyber Pakhtunkhwa, Pakistan. August 22-25, 2016.
33. Participation in ‘**National Symposium on Emerging Trends in Applied Physics**’ by Department of Physics, University of Agriculture Faisalabad-Pakistan, December 3, 2016.
34. Participation in ‘**National Workshop on Technical and Patent Writing**’ by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, January 28th, 2017.
35. Participation in ‘**National Seminar on FT-IR and FT-NIR Applications**’ by Rays Technologies (Bruker) Lahore-Pakistan, February 14, 2017.

36. Participation in “**6th Technical Workshop on Statistical Analysis**” by Department of Chemistry, University of Sargodha, Women Campus Faisalabad-Pakistan, May 06, 2017.
37. **Participation, abstract publication in ‘10th Chemistry Conference 2018 “Chemistry in Engineering and Life Sciences”, at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.**
38. **Participation in “ International Conference on Modern Trends in Chemistry and Energy Technologies” Departments of Chemistry, Pharmacy and Energy Research Center, COMSATS University Islamabad, Lahore Campus-Pakistan, October 22-23 2018.**
39. **Research collaboration visit** to “Institute of Theoretical Chemistry, Jilin University, Changchun, PR China Under “One Road One Belt Project” ” (*Grant # DL20180036 from November 23-30th, 2018 from State Administration of Foreign Expert Affairs of China*) and collaboration bond was signed between “Institute of Theoretical Chemistry, Jilin University and Department of Chemistry, University of Agriculture, Faisalabad, Pakistan.
40. **Participation in ‘2nd international Symposium on Pharmaceutical Sciences at GC University Faisalabad, Pakistan, January 30th, 2019.**
41. **Participation in ‘two day International Symposium” on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.**
42. **Participation in “1st international Conference on Surface Sciences Innovations and Applications for Geoenvironmental Challenges” at Institute of Soil and Environmental Sciences, University of Agriculture Faisalabad, Pakistan, April 25-26, 2019.**
43. **Participation in “One Day Nano-Tech Meeting on Wastewater Treatment” at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3rd, 2019.**
44. **Participation in “Two Days training GCWU May 2019.**
45. **Participation in “One Day Workshop on Fundamentals of Laboratory Biosafety” at Department of Biochemistry, University of Agriculture Faisalabad, Pakistan, Feb 24, 2020.**
46. Participation in “One Day 3rd National Symposium on One Health” at Faculty of Veterinary Sciences, University of Agriculture Faisalabad, Pakistan, Sep 8th, 2021.
47. Participation in “One Day Workshop on Discovering the innovative progressions in catalysis” at Faculty of Sciences, University of Agriculture Faisalabad, Pakistan, Dec 20th, 2021.

48. Participation in “Two Days 1st International Conference on Innovation in Chemistry & Physics at, Department of Chemistry and Physics, University of Education, Faisalabad Campus, Pakistan, March 14-15th, 2022.
49. **Participation** in “International Workshop on Capacity Building of national Scientist and relevant Stakeholders on MRL & Biopesticides” at Department of Entomology, University of Agriculture Faisalabad, Pakistan, Feb 16th, 2023.

ONLINE PARTICIPATION IN DIFFERENT SCIENTIFIC ACTIVITIES

1. **Participation in the National Artificial Intelligence Forum** organized by Sino-Pak Center for Artificial Intelligence (SPCAI), PAF-IASST, Haripur, Pakistan, on 2nd September 2021.
2. **Participation** in a **webinar (via Zoom)** on “Women in Science and Global Health” organized by Department of Pediatrics and Child Health, Aga Khan University, Karachi, Pakistan, on 25th November 2020.
3. **Participation** in a **webinar (via Zoom)** on “Capacity building for launching and Running a Successful Journal” organized by Department of Chemistry, GCWUF on 3rd December 2020.
4. **Participation in a webinar (via Zoom) on ‘Management of Drinking Water, Dams, and Lake Basins Depending on The Changing Climate’ by COMSTECH - March 13, 2025.**
- 5.

ABSTRACT PUBLISHED IN CONFERENCES

1. **Abstract Published Shamsa Bibi, Shafiq-Ur-Rehman and JingPing Zhang, “Theoretical Studies to Investigate the Effect of Different Cores in Two Different Topologies in Donor Materials toward Organic Solar Cells”. Poster and abstract Published in “7th International Conference: Environmentally Sustainable Development – ESDev-VII” August 26-28th 2017.**
2. **Abstract publication in ‘10th Chemistry Conference 2018 “Chemistry in Engineering and Life Sciences”, at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.**
3. **Abstract publication, entitled as “Gemcitabine-Based Anticancer Drug with Metal-Doped BN24 as a Drug Delivery Carrier: Density Functional Theory”, in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.**
4. **Abstract publication, entitled as “Novel Phenolic Compounds as Potential Therapeutic Candidates Against SARS-Cov-2, Using Quantum Chemistry, Molecular Docking and Dynamic Studies: in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.**

5. **Won 3rd Prize & Abstract publication**, entitled as “Novel Phenolic Compounds as Potential Therapeutic Candidates Against SARS-Cov-2, Using Quantum Chemistry, Molecular Docking and Dynamic Studies: in Two Day International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
6. **Abstract publication**, entitled as “Fragmentation Mechanisms Of Secnidazole By Advanced Oxidation Processes: DFT Study”, in Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
7. **Abstract publication**, entitled as “Adsorption And Removal Of Manganese And Vanadium From Wastewater By Graphene Oxide /Chitosan Composites; A Computational Study”, in Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
8. **Abstract publication**, entitled as “A DFT Study Of Solvent Impact On The Photochemical Properties Of Anticancer Drugs PLX4720”, In Three Days “International Conference on “Recent Advances in Interdisciplinary Natural Sciences”, organized by Department of Chemistry, Government College Women University, Faisalabad, Jan 27-28th, 2022.
9. **Abstract publication**, entitled “*Innovative Computational Approaches for Designing Advanced Optoelectronics Materials towards Energy Applications*”, in the 4th International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by the Department of Chemistry, Government College Women University, Faisalabad, December 4-6th, 2024.
10. **Abstract publication**, entitled “*Computational Analysis of Ribofuranose Nucleoside Derivatives: Targeting EGFR and VEGFR2 in Cancer Cells*”, in the 4th International Conference on “Recent Advances in Interdisciplinary Sciences”, organized by the Department of Chemistry, Government College Women University, Faisalabad, December 4-6th, 2024.
11. **Won 3rd prize in poster & Abstract publication**, entitled “*Modeling 3Bha Adsorption on Polyethylene and Polypropylene Microplastics*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
12. **Abstract publication**, entitled “*Exploring Symmetry in Curcuminoids Derivatives for Performance of Photovoltaic Materials*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
13. **Abstract publication**, entitled “*Exploring the Anticancer Potential of Ribofuranose Nucleosides: A Combined DFT and Docking Study*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to

Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.

14. **Abstract publication**, entitled “*Designing the Electron Push-Pull Chromophores for Efficient Nonlinear Optical And Photovoltaic Properties*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
15. **Abstract publication**, entitled “*Computational Studies of Phenothiazine-Based Derivatives for Fluorescent Applications in Semiconductors*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
16. **Abstract publication**, entitled “*Multicomponent Composite for Dye Remediation: Cellulose, Clay, and Sodium Alginate - A Combined Experimental and DFT Investigation*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
17. **Abstract publication**, entitled “*The Impact of Nanostructures on Targeted Drug Delivery of Anticancer Drugs using DFT Studies*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
18. **Abstract publication**, entitled “*Optimizing Optoelectronic Properties of Quinoidal Oligomers Through Shape, Size, and Heteroatom Substitution*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
19. **Abstract publication**, entitled “*Quantum Chemical Approaches for Designing High-Performance Ladder-Shaped NLO Molecules*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
20. **Abstract publication**, entitled “*Superalkali X_3O ($X = Li, Na, K$) Doped $B_{12}N_{12}$ Nano-Cages as a New Drug Delivery Platform for Chlormethine: A DFT Approach*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
21. **Abstract publication**, entitled “*Computational Study of BC_3 Graphene Interaction with Amantadine for Sensing Applications*”, in Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.
22. **Abstract publication**, entitled “*Twisted Small Molecule Donors with Enhanced Intermolecular Interactions Towards Efficient all Small-Molecule Organic Solar Cells*”, in

Two Day International Conference on “Functional Materials and Emerging Technologies; Integrating Materials Science to Community Needs”, organized by the Department of Chemistry, University of Agriculture, Faisalabad, November 25-26th, 2024.