# DR. SHAFIQ UR REHMAN

Ph.D. Chemistry (Jilin University PR China)
Post Doc. (Chinese Academy of Sciences, PR China)



## **SUMMARY**

Highly motivated and results-oriented scholar with a strong background in the subject of chemistry and nine years of teaching and research experience as an Assistant Professor and Post-doc scholar. Expertise in teaching courses at the BS and M. Phil /PhD level. Proven ability to develop engaging curriculum, foster a stimulating learning environment, and achieve strong student outcomes. Demonstrated research productivity with high impact factor publications in peer-reviewed journals.

### **AREAS OF RESEARCH**

• Computational Chemistry

#### **EDUCATION**

•	Ph.D. in Chemistry Jilin University, PR China	2009-2013
•	Master of Science in Chemistry University of the Punjab, Lahore, Pakistan	2001-2003
•	Bachelor of Science University of the Punjab, Lahore Pakistan	1999-2001
WORK		
•	Assistant Professor Chemistry Department, University of Agriculture Faisalabad (UAF)	2015- 2024
•	Research Associate Alan G. MacDiarmid Institute, Jilin University, Changchun, PR China	2014-2015
•	Postdoctoral Researcher	2013-2014

# SCHOLARSHIPS AND AWARDS

Sciences, Changchun, PR China

**Research Chemist (Paper & Board Mills)** 

- Cultural Exchange Scholarship (Ph.D.), Ministry of Education, Pakistan 2008
- Chinese Government Scholarship (Ph.D.), Jilin University, PR China
- CAS Fellowship for Postdoctoral and Visiting Scholars from Developing Countries 2013. The Chinese Academy of Sciences, PR China

Changchun Institute of Applied Chemistry (CIAC), Chinese Academy of

Research & Development Department, Packages Ltd. Lahore, Pakistan

# **COMPUTATIONAL SKILLS**

•	Gaussian 09 / 16	•	Q Series TA Thermal Analysis	•	ChemDraw
•	GaussView 6	•	PyMolyze	•	OriginPro

2004-2008

GaussSumMercuryEndNote

### ADMINISTRATIVE AND ADVISORY DUTIES

- Hall Superintendent, Khalid Hall, UAF, Faisalabad (2016-2023)
- Tutor , Tutorial Group TG-6 Waris , UAF , Faisalabad (2016-2024)
- Deputy DSA, DSA Office UAF, Faisalabad (2016-2022)

#### RESEARCH PROJECTS AND GRANTS

- SRGP PROJECT by HEC, Pakistan Co-Principal Investigator
- Collaborative research project entitled "The Experimental and Computational Study of Optical and Nonlinear Optical Materials Using State-of-the-art Chemical Methods (Project No. RGP. 2/272/44) approved by Deanship of Scientific Research, King Khalid University, Ministry of Education, Kingdom of Saudi Arabia.
- Collaborative research project entitled "Innovative design of molecular materials in organic photovoltaic devices." (Project No DL20180036.) funded by Jilin University ,Ministry of Education PR China.

# RESEARCH SUPERVISION

Program	Supervisor	<b>Supervisory Committee</b>	<b>Total students</b>
M. Phil Chemistry Thesis	91	40	131
MSc Chemistry Tech. Report	31	-	31

# **BOOK CHAPTERS**

- 1. Haq Nawaz Bhatti and Saima Noreen, 2017. Principles of Environmental Chemistry. The Caravan Book House Lahore (Chapter # 02- Atmospheric Chemistry).
- 2. 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).

### **PATENTS**

1. Janjua, Mohammad Ramzan Saeed Ashraf, Saba Jamil, Hasnaat Ahmad, **Shafiq Ur-Rehman**, and Shanza Rauf Khan. "Graphene oxide and cobalt tin oxide nanocomposite and method of use." U.S. Patent 10,882,029 issued January 5, **2021**.

# **PUBLICATIONS**

Total No. of **Publications** = **49**Total **Impact Factor** = ~ **166**No. of Publications as **Principal Author** = **32**HJRS -W **Category** Publications = **21** 

1. Muhammad, S., Faiz, A., Bibi, S., **Shafiq urRehman** & Alshahrani, M. Y. (2024). 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*, 108218. (**IF =2.6**)

- 2. Bibi, Shamsa, Iqra Kaifi, Shabbir Muhammad, **Shafiq urRehman**, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, and Aijaz Rasool Chaudhry. "Quantum chemical framework for designing high-performance ladder-shape NLO molecules and study of implicit vs explicit solvent effects on their NLO properties." *Journal of Molecular Liquids* (2024): 125298. (**IF =5.3**)
- 3. Bibi, Shamsa, Aamna Imtiaz, Shabbir Muhammad, **Shafiq urRehman**, Aijaz Rasool Chaudhry, Abdullah G. Al-Sehemi, Bakhet Ahmad Alqurashy, and Mazhar Amjad Gilani. "Tailoring the donor moieties in TPA-based organic dyes for efficient photovoltaic, optical and nonlinear optical response properties." *International Journal of Quantum Chemistry* 124, no. 7 (2024): e27362. (IF =2.2, HJRS=X)
- 4. Muhammad, Shabbir, Nimra Zahir, Shamsa Bibi, Mohammad Y. Alshahrani, ShafiqurRehman, Aijaz Rasool Chaudhry, Fatima Sarwar, and 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* 109 (2024): 108020. (IF =3.1, HJRS=X)
- 5. **Shafiq UrRehman,** Hammad Aslam, Shamsa Bibi, Nazish Jahan, Muhammad Irfan Majeed, Haq Nawaz, Samreen Gul Khan, and Hong-Xing Zhang. "Tuning of end-groups in diketopyrrolopyrrole-based acceptors molecules for organic photovoltaics." *Sustainable Chemistry for the Environment* 5 (2024): 100068. (IF =1, HJRS=)
- 6. Muhammad, Shabbir, Sadia Riaz, **Shafiq urRehman**, Shamsa Bibi, Abdullah G. Al-Sehemi, H. Algarni, and Aijaz Rasool Chaudhry. "Understanding the role of symmetric/asymmetric curcuminoids in designing efficient optical, nonlinear optical and photovoltaic materials." *Optical and Quantum Electronics* 56, no. 4 (**2024**): 681. (**IF** =**3**, **HJRS=W**)
- 7. Muhammad, Shabbir, **Shafiq UrRehman**, Maimoona Zia, Shamsa Bibi, Muhammad Imran Tousif, Aftab Hussain, Tareg M. Belali, and 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* (**2024**): 137744. (**IF =3.8, HJRS=**)
- 8. **Shafiq urRehman**, Sajjad, Ayesha, Shamsa Bibi, Hira Tabassum, Saba Jamil, Shanza Rauf Khan, Nadia Munawar, Asim Mansha, Sadia Asim, and Hong-Xing Zhang. "A DFT study on removal of Mn and V from wastewater using chitosan/graphene oxide composite as adsorbent." *Chemistry of Inorganic Materials* (2023): 100030. (IF =0.9, HJRS=)
- 9. Bibi, Shamsa, Gulzaib Basharat, Saba Jamil, **Shafiq urRehman**, Shanza Rauf Khan, Aftab Hussain, and Ran Jia. "Solvent impact on the photochemical properties of anticancer drug PLX4720; a computational study." *Inorganic Chemistry Communications* 157 (**2023**): 111424. (**IF = 3.42, HJRS=X**)
- 10. BiBi, Shamsa, Zarina Kousar, **Shafiq-ur-Rehman**, Ijaz Ahmad Bhatti, Haq Nawaz Bhatti, Shanza Rauf Khan, Fu-Quan Bai, and Gohar Farid. "Newly efficient designed benzothiadiazole (ADADA topology) based materials for organic photovoltaics: DFT Study." *Materials Today Communications* 36 (**2023**): 106481. (**IF =3.66**, **HJRS=W**)
- 11. Bibi, Shamsa, Aamna Saleem, **Shafiq ur Rehman**, Ijaz Ahmad Bhatti, Muhammad Adnan Iqbal, Shahid Bashir, Bai Fu Quan, and Raziya Nadeem. "DFT study of oxidation mechanism of secnidazole as an emerging contaminant: Application as STI control." *Journal of Physical Organic Chemistry* 36, no. 4 (**2023**): e4480. (**IF =2.2 , HJRS=X**)
- 12. Naz, Saman, Guria Bibi, Saba Jamil, **Shafiq UrRehman**, Shamsa Bibi, Sarmed Ali, Tahreem Khan, Shanza Rauf Khan, and Muhammad Ramzan Saeed Ashraf Janjua. "Preparation of manganese-doped tin oxide nanoparticles for catalytic reduction of organic dyes." *Chemical Physics Letters* 802 (**2022**): 139768. (**IF =2.33 , HJRS=X**)
- 13. Munawar, Khurram Shahzad, Saqib Ali, Abdur Rauf, Shamsa Bibi, Muhammad Ashfaq,

- Muhammad Nawaz Tahir, **Shafiq urRehman**, and Lubna Rasool. "Structural and computational analysis, spectroscopic and electrochemical elucidation of a Schiff base." *Journal of the Iranian Chemical Society* 19, no. 9 (**2022**): 3845-3860. (**IF =2.64 , HJRS=X**)
- 14. Muhammad, Shabbir, Amna Bibi, **Shafiq-urRehman**, Shamsa Bibi, Abdullah G. Al-Sehemi, H. Algarni, and Fatima Sarwar. "Exploring the quinoidal oligothiophenes to their robust limit for efficient linear and nonlinear optical response properties." *Chemical Papers* 76, no. 7 (2022): 4273-4288. (**IF** =2.1, **HJRS=X**)
- 15. UlAin, Qurat, Sarmed Ali, Saba Jamil, Shamsa Bibi, Shanza Rauf Khan, **Shafiq UrRehman**, Guria Bibi et al. "Comparison of catalytic and fuel additive properties of bimetallic nanoparticles and its composite: FeMnO3 and PANI-FeMnO3." *Materials Science in Semiconductor Processing* 144 (**2022**): 106630. (**IF** =**4.64**, **HJRS=W**)
- 16. Mansha, Asim, Syeda Anam Asad, Sadia Asim, Shamsa Bibi, **Shafiq-Ur Rehman**, and Alina Shahzad. "Review of recent advancements in fluorescent chemosensor for ion detection via coumarin derivatives." *Chemical Papers* 76, no. 6 (2022): 3303-3349. (IF =2.1, HJRS=X)
- 17. Kausar, Abida, **Shafiq Ur Rehman**, Farwa Khalid, Adrián Bonilla-Petriciolet, Didilia Ileana Mendoza-Castillo, Haq Nawaz Bhatti, Sobhy M. Ibrahim, and Munawar Iqbal. "Cellulose, clay and sodium alginate composites for the removal of methylene blue dye: Experimental and DFT studies." *International Journal of Biological Macromolecules* 209 (**2022**): 576-585. (**IF =8.2**, **HJRS=W**)
- 18. Sarwar, Fatima, Shabbir Muhammad, **Shafiq Ur Rehman**, Shamsa Bibi, Abdullah G. Al-Sehemi, H. Algarni, and Santosh Kumar. "Insighting the systematic impact of shape, size and substitution of heteroatoms in quinoidal oligomers to tune their optoelectronic properties." *Optical and Quantum Electronics* 54, no. 6 (**2022**): 356. (**IF =3 , HJRS=W**)
- 19. Majeed, Sana, **Shafiq Ur Rehman**, Muhammad Anjum Zia, and Javed Iqbal. "Tuning the optoelectronic properties of cross conjugated small molecules using benzodithiophene as a core unit with favorable photovoltaic parameters: a DFT study." *Journal of Physics D: Applied Physics* 55, no. 29 (**2022**): 295106. (**IF =3.48, HJRS=W**)
- 20. Perveen, Shazia, Raziya Nadeem, **Shafiq ur Rehman**, Nosheen Afzal, Shazia Anjum, Saima Noreen, Rashid Saeed, Mongi Amami, Samiah H. Al-Mijalli, and Munawar Iqbal. "Green synthesis of iron (Fe) nanoparticles using Plumeria obtusa extract as a reducing and stabilizing agent: Antimicrobial, antioxidant and biocompatibility studies." *Arabian Journal of Chemistry* 15, no. 5 (2022): 103764. (IF =6.72, HJRS=W)
- 21. Muhammad, Shabbir, **Shafiq Urrehman**, Fatima Sarwar, Shamsa Bibi, Raziya Nadeem, Muhammad Waheed Mushtaq, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, and Sajjad Hussain. "Insighting the functionally modified C60 fullerenes as an efficient nonlinear optical materials: A quantum chemical study." *Materials Science in Semiconductor Processing* 141 (**2022**): 106421. (**IF =4.64, HJRS=W**)
- 22. **UrRehman, Shafiq**, Makhvela Anwer, Shamsa BiBi, Saba Jamil, Muhammad Yasin, Shanza Rauf Khan, Raziya Nadeem, Sarmed Ali, and Ran Jia. "DFT analysis of different substitutions on optoelectronic properties of carbazole-based small acceptor materials for Organic Photovoltaics." *Materials Science in Semiconductor Processing* 140 (**2022**): 106381. (**IF =4.64**, **HJRS=W**)
- 23. Bibi, Shamsa, **Shafiq Ur-Rehman**, Laryeb Khalid, Ijaz Ahmad Bhatti, Haq Nawaz Bhatti, Javed Iqbal, Fu Quan Bai, and Hong-Xing Zhang. "Investigation of the adsorption properties of gemcitabine anticancer drug with metal-doped boron nitride fullerenes as a drug-delivery carrier: a DFT study." *RSC advances* 12, no. 5 (**2022**): 2873-2887. (**IF =3.9 , HJRS=W** )
- 24. Bibi, Shamsa, Shafiq Urrehman, Laryeb Khalid, Muhammad Yaseen, Abdul Quyyam Khan,

- and Ran Jia. "Metal doped fullerene complexes as promising drug delivery materials against COVID-19." *Chemical Papers* 75, no. 12 (**2021**): 6487-6497. (**IF =2.2 , HJRS=X** )
- 25. Bibi, Shamsa, Faiza Farooq, **Shafiq UR Rehman**, Fu Quan Bai, and Hong-Xing Zhang. "DFT and TD-DFT studies of phenothiazine-based derivatives as fluorescent materials for semiconductor applications." *Materials Science in Semiconductor Processing* 134 (**2021**): 106036. (**IF =4.64**, **HJRS=W**)
- 26. Yaqoob, Umer, Sidra Rafiq, **Shafiq UR Rehman**, Shamsa Bibi, and Javed Iqbal. "Designing and comparative analysis of 3D subphthalocyanines based non-fullerene acceptor molecules as an efficient material for organic solar cells." *Optik* 246 (2021): 167845. (IF =3.1, HJRS=W)
- 27. Bibi, Amna, 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* 6, no. 38 (**2021**): 24602-24613. (**IF =4.1 , HJRS=W**)
- 28. Zia, Maimoona, Shabbir Muhammad, **Shafiq ur-Rehman**, Shamsa Bibi, Sumra Wajid Abbasi, Abdullah G. Al-Sehemi, Aijaz Rasool Chaudhary, and 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* 43 (**2021**): 128079. (**IF =2.7 , HJRS=X**)
- 29. Bibi, Shamsa, Mehwish Khan, **Shafiq ur-Rehman**, Muhammad Yaseen, Shabbir Muhammad, Raziya Nadeem, Nazish Jahan, Saima Noreen, and 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* 34, no. 6 (**2021**): e4183. (**IF** =1.8, **HJRS=X**)
- 30. Shoaib, Muhammad, **Shafiq Ur-Rehman**, Shamsa Bibi, Inam Ullah, Saba Jamil, Javed Iqbal, Asma Alam, Ushna Saeed, and 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* 235, no. 4 (**2021**): 427-449. (**IF** =**2.5**, **HJRS=NIL**)
- 31. **Shafiq Ur-Rehman**, Ghafoor, Shaista, Shamsa BiBi, Abida Kausar, Shaukat Ali, Sadia Asim, Asim Mansha, Syeda Aaliya Shehzadi, and Ran Jia. "Dft and TDDFT studies of non-fullerene organometallic based acceptors for organic photovoltaics." *Journal of Inorganic and Organometallic Polymers and Materials* 31 (**2021**): 1676-1687. (**IF =4 , HJRS=W** )
- 32. Janjua, Mohammad Ramzan Saeed Ashraf, Saba Jamil, Hasnaat Ahmad, **Shafiq Ur-Rehman**, and Shanza Rauf Khan. "Graphene oxide and cobalt tin oxide nanocomposite and method of use." U.S. Patent 10,882,029, issued January 5, **2021**. (**IF** = , **HJRS**= )
- 33. Yaseen, Muhammad, Muhammad Dilawar, Hina Ambreen, Shamsa Bibi, **Shafiq Ur Rehman**, Umair Shahid, Mehwish Khalid Butt, Abdul Ghaffar, and Adil Murtaza. "Electronic, optical and magnetic properties of low concentration Ni-doped CdSe by first principle method." *Bulletin of Materials Science* 43 (**2020**): 1-8. (**IF =1.8 , HJRS=NIL** )
- 34. Irfan, Muhammad, Rabia Rehman, Mohd R. Razali, **Shafiq-ur Rehman** and Muhammad Adnan Iqbal. "Organotellurium compounds: an overview of synthetic methodologies." *Reviews in Inorganic Chemistry* 40, no. 4 (**2020**): 193-232. (**IF =4.1, HJRS=X**)
- 35. Saeed, Aqsa, Shabbir Muhammad, **Shafiq-ur Rehman**, Shamsa Bibi, Abdullah G. Al-Sehemi, and Muhammad Khalid. "Exploring the impact of central core modifications among several push-pull configurations to enhance nonlinear optical response." *Journal of Molecular Graphics and Modelling* 100 (**2020**): 107665. (**IF =2.9 , HJRS=X**)
- 36. UrRehman, Shafiq, Asma Alam, Shamsa Bibi, Sana Sadaf, Shanza Rauf Khan, Muhammad

- Shoaib, Abdul Qayyum Khan, Mehwish Khan, and Waheed UrRehman. "The effect of different aromatic conjugated bridges on optoelectronic properties of diketopyrrolopyrrole-based donor materials for organic photovoltaics." *Journal of Molecular Modeling* 26 (2020): 1-16. (IF =2.2, HJRS=X)
- 37. Yaseen, Muhammad, Hina Ambreen, Abu Sufyan, Mehwish Khalid Butt, **Shafiq UrRehman**, Javed Iqbal, Misbah, Shamsa Bibi, Adil Murtaza, and Shahid M. Ramay. "Optical and magnetic properties of manganese doped zinc sulphide: density functional theory approach." *Ferroelectrics* 557, no. 1 (2020): 112-122. (**IF** =0.8, **HJRS=Y**)
- 38. Yaseen, Muhammad, Amna Ashfaq, **Shafiq Ur Rehman**, Anam Akhtar, Rida Asghar, Hina Ambreen, Mehwish Khalid Butt, Saima Noreen et al. "Investigation of LaAlO3 pervoskite compound for optoelectronic and thermoelectric devices under pressure." *Materials Research Express* 7, no. 1 (2020): 015907. (IF =2.3, HJRS=X)
- 39. Yaseen, M., H. Ambreen, U. Shoukat, M. Butt, S. Noreen, **S. Rehman**, and S. M. Ramay. "Investigation of Cr doped CdTe for optoelectronic and spintronic devices applications." *J. Ovonic Res* 15, no. 6 (2019): 401-409. (IF =1.16, HJRS=Y)
- 40. Waqas, Ahmad, Shamsa Bibi, **Shafiq-ur Rehman**, Sufian Afzal, Muhammad Yaseen, Muhammad Shoaib, Ushna Saeed, and 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* 32, no. 11 (**2019**): e4000. (**IF =1.8 , HJRS=X** )
- 41. Bibi, Shamsa, **Shafiq-ur-Rehman**, Ran Jia, Hong-Xing Zhang, and 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* 186 (**2019**): 311-322. (**IF =6.7, HJRS=W**)
- 42. Saeed, Ushna, Shamsa Bibi, **Shafiq ur-Rehman**, Shanza Rauf khan, Muhammad Shoaib, Muhammad Adnan Iqbal, Faisal Nawaz, and Ran Jia. "Designation and Match of Non-Fullerene Acceptors with X-Shaped Donors toward Organic Solar Cells." *ChemistrySelect* 4, no. 13 (2019): 3654-3664. (IF =2.1, HJRS=X)
- 43. Jamil, Saba, Hasnaat Ahmad, Shanza Rauf Khan, **Shafiq Ur Rehman** and Muhammad Ramzan Saeed Ashraf Janjua. "The first morphologically controlled synthesis of a nanocomposite of graphene oxide with cobalt tin oxide nanoparticles." *RSC advances* 8, no. 64 (**2018**): 36647-36661. (**IF** = **3.9**, **HJRS=W**)
- 44. Wei, Ji Hai, Zhao Xiao Gang, Li Qing Ming, **Shafiq urRehman**, Zhou Hong Wei, Dang Guo Dong, and Chen Chun Hai. "Atomic oxygen resistant phosphorus-containing copolyimides derived from bis [4-(3-aminophenoxy) phenyl] phenylphosphine oxide." *Polymer Science Series B* 56 (**2014**): 788-798. (**IF =1.2 , HJRS=NIL** )
- 45. **UrRehman, Shafiq**, GuangLiang Song, He Jia, HongWei Zhou, XiaoGang Zhao, GuoDong Dang, and ChunHai Chen. "Synthesis and characterization of benzimidazole-based low CTE block copolyimides." *Journal of Applied Polymer Science* 129, no. 5 (**2013**): 2561-2570. (**IF** =3, **HJRS=W**)
- 46. Ali, Imtiaz, **Shafiq UrRehman**, Syed Hyder Ali, and Asad Javaid. "The effect of borax-modified starch on wheat straw-based paper properties." *Journal of Applied Polymer Science* 128, no. 6 (**2013**): 3672-3677. (**IF =3 , HJRS=W**)
- 47. Xiaohui Yu, Daming Wang, Xiaogang Zhao, Dong Yang, **Shafiq urRehman**, Chunhai Chen, Hongwei Zhou, Guodong Dang. "High modulus and high strength ultra-thin polyimide films with hot-stretch induced molecular orientation." Materials Chemistry and Physics 139, no. 2-3 (2013): 968-974. (**IF** =4.6, **HJRS**= **W**)

- 48. **Shafiq-ur-Rehman**, Peng Li, HongWei Zhou, XiaoGang Zhao, GuoDong Dang, ChunHai Chen. "Thermally and hydrolytically stable polyimides containing naphthalimide units." *Polymer degradation and stability* 97, no. 9 (**2012**): 1581-1588. (**IF** =**5.9**, **HJRS**= **W**)
- 49. S.A.I. Bokhari, M.I. Rajoka, A. Javaid, **Shafiq-ur-Rehman**, Ishtiaq-ur-Rehman, F. Latif. "Novel thermodynamics of xylanase formation by a 2-deoxy-d-glucose resistant mutant of Thermomyces lanuginosus and its xylanase potential for biobleachability." *Bioresource technology* 101, no. 8 (**2010**): 2800-2808. (**IF** =**11.9**, **HJRS**= **W**)

# CONFERENCES/WORKSHOPS/ REFRESHER COURSES

- 1. 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.
- 2. Participation in "One Day Nano-Tech Meeting on Wastewater Treatment" at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3rd, 2019.
- 3. As a member of the "Organizing Committee" in "One Day Nano-Tech Meeting on Wastewater Treatment" at Department of Chemistry, University of Agriculture Faisalabad, Pakistan, May 3rd, 2019.
- 4. Participation in "Two Days training GCWU May 2019.
- Oral Presentation and Abstract publication in 'The Seventeenth International Symposium on Electroanalytical Chemistry & The Third International Meeting on Electrogenerated 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.
- 6. Participation in international training on "Recent Advances in Computational Chemistry" at Institute of Theoretical Chemistry, Jilin University Changchun 130023, China, Aug 08-21, 2019.
- 7. 18th National Chemistry Conference, Institute of Chemistry, University of the Punjab, Lahore, Chemical Society of Pakistan, Feb. 2008.
- 8. International Conference on Computational Chemistry and Biology (ICCCB) November 2012 Shenzhen, China.
- 9. International Conference on Theoretical and High-Performance Computational Chemistry 2012, Nanjing, China
- 10. 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.
- 11. The 12th National Conference of Quantum Chemistry (NCQC), Taiyuan, China, June 2014.
- 12. Participation in 'National Grant Writing Workshop' by US-Pakistan Center for Advanced Studies in Agriculture and Food Security (USPCAS-AFS) at UAF, April 6-7, 2016.
- 13. 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.
- 14. Participation in 'International Conference on Energy for Environmental and Economic Sustainability (ICEEES2016)' Lahore, Pakistan October 20 23, 2016.

- 15. Participation in '27th National and International Chemistry Conference at Department of Chemistry, University of Malakand, Khyber Pakhtunkhwa, Pakistan. August 22-25, 2016.
- 16. Participation in 'National training Workshop on X-ray Crystallography' by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, November 7-December 2, 2016.
- 17. Participation in 'National Symposium on Emerging Trends in Applied Physics' by Department of Physics, University of Agriculture Faisalabad-Pakistan, December 3, 2016.
- 18. Participation in 'National Workshop on Technical and Patent Writing' by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, January 28th, 2017.
- 19. Participation in 'National Seminar on FT-IR and FT-NIR Applications' by Rays Technologies (Bruker) Lahore-Pakistan, February 14, 2017.
- 20. Participation in '4th International Conference on Global Environmental Changes' GC Participation in a two days 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.
- 21. Participation in "6th Technical Workshop on Statistical Analysis" by Department of Chemistry, University of Sargodha, Women Campus Faisalabad-Pakistan, May 06, 2017.
- 22. 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.
- 23. Abstract publication and Oral Presentation in '7th International Conference "Environmentally Sustainable Development", ESDev-2017 at CIIT Abbottabad, Pakistan, August 26-28, 2017.
- 24. Participation and acting as Organizer in National Workshop "2nd Workshop on Advanced Chemical Techniques in Natural and Applied Sciences" by Department of Chemistry, University of Agriculture Faisalabad-Pakistan, September 18-20, 2017.
- 25. Participation, abstract publication in '10th Chemistry Conference 2018 "Chemistry in Engineering and Life Sciences", at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.
- 26. 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.
- 27. 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.
- 28. 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.
- 29. Research collaboration visit to "Institute of Theoretical Chemistry, Jilin University, Changchun, PR China Under "One Road One Belt Project" "from November 23-30th, 2018 and MOU was signed between "Institute of Theoretical Chemistry, Jilin University and Department of Chemistry, University of Agriculture, Faisalabad, Pakistan.
- 30. Member of Organizing Committee in National Workshop "Academic writing skills" by Community College, University of Agriculture Faisalabad-Pakistan, December 27, 2018.

- 31. Participation in '2<sup>nd</sup> international Symposium on Pharmaceutical Sciences at GC University Faisalabad, Pakistan, January 30th, 2019.
- 32. Acted as member of "Poster management committee" for "two-day International Symposium" on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.
- 33. 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.
- 34. As a member of "organizing Committee" in 'two-day International Symposium" on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06- 07, 2019.
- 35. Participation in 'two-day International Symposium" on Technologies and Materials for Renewable Energy, Environment and Sustainability, Department of Chemistry, UAF, Feb 06-07, 2019.
- 36. 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. 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.
- 37. Abstract Published Shamsa Bibi, Shafiq-Ur-Rehman and Jinping 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.
- 38. Abstract publication in '10th Chemistry Conference 2018 "Chemistry in Engineering and Life Sciences", at Chemistry Division PINTECH, Islamabad, Pakistan, August 07-09, 2018.
- 39. The 9th China-Japan Symposium on Advanced Aromatic Polymers, Shanghai 2010
- 40. The Fourth International Symposium on Engineering Plastics, Beijing 2009
- 41. International Symposium on Fine Chemistry and Functional polymers, Shanghai 2011
- 42. "ISO 14001:2004 EMS Internal Auditing", SGS Pakistan 2005
- 43. "Biological wastewater treatment" Papierzentrum Gernsbach-Germany, Lahore 2007
- 44. "Problem Solving and Decision-Making Skills", Pakistan Institute of Management, Lahore 2005
- 45. "Project Monitoring, Control & Evaluation", Pakistan Institute of Management, Lahore 2006