

# RAO AQIL SHEHZAD



## Summary

Mr. Rao Aqil Shehzad has completed his matric degree from BISE Lahore, an intermediate degree from BISE Sahiwal, and a bachelor's degree from the University of Education, Lahore, Okara Campus, Pakistan. He did his MS/MPhil and PhD from the University of Agriculture, Faisalabad, Pakistan, focusing on the design and fabrication of Organic Functional Materials under the supervision of Associate Prof. Dr Javed Iqbal. From MS, he worked as a Research Trainee and Teaching Assistant (TA) at the Department of Chemistry, University of Agriculture, Faisalabad, Pakistan, under the supervision of Associate Prof. Dr Javed Iqbal in collaboration with Assistant Prof. Dr Muhammad Shabbir, King Khalid University, Abha, Kingdom of Saudi Arabia. He is President of chemical society in UAF and visiting lecturer in University of Okara. He worked as a Research Associate at the UET-Faisalabad campus in NRPU Project no. 16544. He also working with Prof. Dr Khurshid Ayub, COMSATS University Islamabad, Pakistan, and Assistant Prof. Dr Riaz Hussain, University of Okara, Pakistan. His current research interests are as follows:

### Organic photovoltaics, Organic electronics & Sensors

Design and synthesis of Photovoltaic (PV) materials and fabrication of solar cells. Design of proficient materials for nonlinear optical applications. Furthermore, design deep fluorescent AIE (aggregation-induced emission) materials for OLED and biosensors application. Study the mechanism and factors affecting aggregation-induced emission.

### Linear and Nonlinear optical materials

Design of Linear and Nonlinear optical (LO and NLO) materials. Design of proficient materials for nonlinear optical polarizability and susceptibility. Implement nonlinear phenomena and investigation from the molecular to the bulk level.

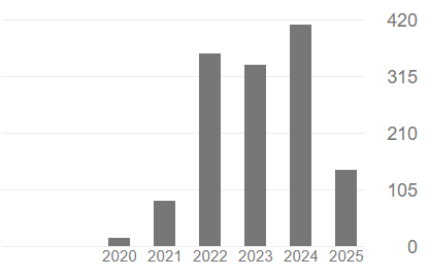
### Computational and Material Chemistry

A computational approach to design molecules based on our organic chemistry knowledge and determine their physical and electronic properties. After careful assessment of the optoelectronic properties, only the desired compounds are synthesized.



#### Cited by

	All	Since 2020
Citations	1351	1350
h-index	21	21
i10-index	31	31



## Personal information

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[Raoaqil.Shehzad@uaf.edu.pk](mailto:Raoaqil.Shehzad@uaf.edu.pk)

Phone: +92 302 4917771

Book Chapter Publication: 1

Research Publications: 46

Impact Factor: 135.3

Age: 29 years

## Language

English: B2 (Proficient)



## Work Experience

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- University of Agriculture, Faisalabad, Pakistan – *Lecturer* (2024 – cont.)  
Constituent College Depalpur, Okara
- University of Agriculture, Faisalabad, Pakistan – *PhD* (2021 – 2024)  
Assisting research activities in the synthetic and computational chemistry labs.
- University of Engineering and Technology, Faisalabad, Pakistan – *Research Associate* (2022 – 2023)  
Worked as a Research Associate in "Carbon nano structures-based photocatalytic device for smog reduction" (HEC funded NRPUR Project No. 16544).
- University of Agriculture, Faisalabad, Pakistan  
*PhD Chemistry, Teaching Assistant (TA)* (2021 – 2022)  
Maintain lab work in Theoretical and Computational Chemistry Laboratory, UAF, Faisalabad



## Education

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- University of Agriculture, Faisalabad, Pakistan  
*PhD* (3.86/4.00; 81%)  
Computational and Theoretical Chemistry Laboratory, UAF, Faisalabad 2021-2025
- University of Agriculture, Faisalabad, Pakistan  
*MS/MPhil* (3.90/4.00; 82%)  
Computational and Theoretical Chemistry Laboratory, UAF, Faisalabad 2018-2020
- University of Education, Lahore, Pakistan  
*BS Honor Chemistry* (3.49/4.00; 79%) 2014-2018
- Board of Intermediate and Secondary Education (BISE) Sahiwal  
*FSc* (80%) Pre-Medical 2012-2014
- Board of Intermediate and Secondary Education (BISE) Lahore  
*Matric* (87%) Science 2010-2012



## Publications

### Book Chapter

1. **Rao Aqil Shehzad**, Saba Zahid, Alvina Rasool, Javed Iqbal. "Organic Semiconductors for Photovoltaics". In: Gupta, R. (eds) Handbook of Energy Materials. Springer (2022), Singapore. [https://doi.org/10.1007/978-981-16-4480-1\\_66-1](https://doi.org/10.1007/978-981-16-4480-1_66-1).

### Optoelectronic properties (Organic Photovoltaics & Nonlinear Optics)

1. Ijaz Ullah, Yunbin Li, **Rao Aqil Shehzad**, Javed Iqbal, and Ezzat Khan. "Synthesis, Crystal Growth, Structural Characterization, Supramolecular Chemistry, and Theoretical Calculations of Methylenium Salts of Benzenesulfonates." *ChemistrySelect* 9, no. 17 (2024): e202401272.
2. Mariam Ishtiaq, Muhammad Salim Akhter, **Rao Aqil Shehzad**. "Structural modification of ACA configured X-PCIC acceptor molecule for efficient photovoltaic properties with low energy loss in organic solar cells." *Journal of Molecular Graphics and Modelling* (2024) 129: 108722.
3. Qundeel, Muhammad Adnan, Riaz Hussain, **Rao Aqil Shehzad**, Shabbir Muhammad, Ghulam Mustafa, Zobia Irshad. "Impact of End-capped Engineering on the Optoelectronic Characteristics of Pyrene-based Non-fullerene Acceptors for Organic Photovoltaics" *International Journal of Quantum Chemistry* (2024) 124(5): e27344.
4. Mehreen Ashiq, **Rao Aqil Shehzad**, Javed Iqbal, Khurshid Ayub. "Sensing applications of graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) for sensing SO<sub>2</sub> and SO<sub>3</sub> – A DFT study". *Physica B* (2024) 676: 415661.
5. Raheela Sharafat, **Rao Aqil Shehzad**, Muneerah Alomar, Rabia Shakeel, Tayyba Khalid, Javed Iqbal, and Rasheed Ahmad Khera. "End-capped engineering of carbazole based dopant free hole transporting material with improved power conversion efficiency." *Optik* (2023) 295: 171537.
6. Khalid, Urooj, **Rao Aqil Shehzad**, *et al.*, "Molecular Engineering of Tetraphenyl-Based Hole Transporting Materials to Enhance Photovoltaic Properties of Perovskite Solar Cells." *Optik* (2023) 295: 171501.
7. Mahmood, Muhammad Saad, **Rao Aqil Shehzad**, and Javed Iqbal. "Sensing applications of graphitic carbon nitride (C<sub>6</sub>N<sub>8</sub>) for Nitrogen oxides: A DFT study." *Physica Scripta* (2023) 98(12): 125001.
8. Rabia Iftikhar, Rabiya Irshad, Waqar Ali Zahid, Waqas Akram, **Rao Aqil Shehzad**, Shaimaa AM Abdelmohsen, Meznah M. Alanazi, Nabeel Shahzad, and Javed Iqbal. "Designing of fluorine-substituted benzodithiophene-based small molecules with efficient photovoltaic parameters." *Journal of Molecular Graphics and Modelling* (2023) 125: 108588.
9. **Rao Aqil Shehzad**, Riaz Hussain, Javed Iqbal, and Khurshid Ayub. "Quantum chemical study of structural, linear, and nonlinear optical response of pure silver clusters Ag<sub>n</sub> (n= 2–10)." *Materials Science in Semiconductor Processing* 163 (2023): 107558.
10. Shanza Hameed, Muhammad Waqas, Saba Zahid, Shehla Gul, Ahmed M. Shawky, Naifa S. Alatawi, **Rao Aqil Shehzad** et al. "Quantum Chemical Approach of Hexaammine (NH<sub>3</sub>)<sub>6</sub> complexant with alkali and alkaline earth metals for their potential use as NLO materials." *Journal of Molecular Graphics and Modelling* (2023) 123: 108505.
11. **Rao Aqil Shehzad**, Javed Iqbal, Shaikat Ali, Hafeez Anwar "Quantum chemical investigation of Z-shaped heptazethrenes derivatives with detailed structural parameters and singlet fission for photovoltaic applications." *Journal of Molecular Graphics and Modelling* (2023) 121: 108432.
12. Qudsia Sehar Hameed, Khadijah Mohammedsaleh Katubi, **Rao Aqil Shehzad**, Khurshid Ayub, Norah Salem Alsaiani, Javed Iqbal, and M. S. Al-Buriahi. "Exohedrally and endohedrally doped calix-4-pyrrole surface by alkali and alkaline earth metals for potential applications as high-performance NLO materials." *Structural Chemistry* (2022) 34(4): 1469-1488.
13. Nimra Maqsood, Areeba Asif, Abraham Elmushyakhi, Muhammad Ans, **Rao Aqil Shehzad**, Alvina Rasool, Zainab Bibi, Ahmed M. Shawky, and Javed Iqbal. "Environmentally affable and highly efficient donor material based on cyclopentadithiophene (CPDT) framework for remarkable organic solar cells." *Optical Materials* 135 (2023): 113316.
14. Amina Rafique, Hadia Maqbool, **Rao Aqil Shehzad**, Ijaz Ahmad Bhatti, Khurshid Ayub, Abraham Elmushyakhi, Ahmed M. Shawky, and Javed Iqbal. "DFT study of enhancement in nonlinear

- optical response of exohedrally and endohedrally alkaline earth metals (Be, Mg, Ca) doped adamanzane." *International Journal of Quantum Chemistry* 123(6) (2023): e27060.
15. Shehla Gul, Alvina Rasool, Shanza Hameed, **Rao Aqil Shehzad**, Khurshid Ayub, Muhammad Ans, and Javed Iqbal. "Alkaline earth metals (Be, Mg, Ca) doped hexamine complexant with enhanced electronic and nonlinear optical properties." *Journal of Molecular Modeling* 28(12) (2022): 1-15.
  16. Tahreem Tahir, Naila Naeem, Muhammad Ans, Alvina Rasool, **Rao Aqil Shehzad**, Javed Iqbal. "Designing of Difluorobenzene Based Donor Molecules with Efficient Photovoltaic Properties towards High Performance Organic Solar Cells." *Russian Journal of Physical Chemistry A* 96(8) (2022): 1817–1827.
  17. Abid Hussain, N.M.A. Hadia, M.M.Hessien, Rasheed Ahmad Khera, Saba Zahid, **Rao Aqil Shehzad**, Ali Raza Ayub, Khurshid Ayub, Javed Iqbal. "DFT study of super-halogen (Al<sup>7</sup>) doped graphitic carbon nitride (C<sub>2</sub>N) and its nonlinear optical properties." *Journal of Molecular Structure* 1270 (2022): 133910.
  18. Emaan Nadeem, Wisha Akram, **Rao Aqil Shehzad**, Khurshid Ayub, Javed Iqbal, Asma M. Alenad, and T. A. Taha. "Alkaline Earth Metals Doped C<sub>2</sub>N With Enhanced Nonlinear Optical Properties." *Optik* 265 (2022): 169514.
  19. Nigarish Bano, Ijaz Ahmad Bhatti, Qurat ul-Ain, Muhammad Mohsin, **Rao Aqil Shehzad**, and Javed Iqbal. "A DFT study of nonlinear optical response of supersalt (Al (BH<sub>4</sub>)<sub>3</sub>) doped boron nitride." *Journal of Taibah University for Science* 16, no. 1 (2022): 621-631.
  20. Ali Raza Ayub, Umer Yaqoob, Sidra Rafiq, **Rao Aqil Shehzad**, Khurshid Ayub, Javed Iqbal, Hui Li, K. H. Mahmoud, and Khaled A. Elsayed. "A Quantum Chemical Study of Outstanding Structural, Electronic and Nonlinear Optical Polarizability of Boron Nitride (B<sub>12</sub>N<sub>12</sub>) Doped with Super Salt (P<sub>7</sub>BaNO<sub>3</sub>)." *Journal of Inorganic and Organometallic Polymers and Materials* (2022): 1-27.
  21. Iqra Zubair, Rasheed Ahmad Khera, Ayesha Naveed, **Rao Aqil Shehzad**, and Javed Iqbal. "Designing the optoelectronic properties of BODIPY and their photovoltaic applications for high performance of organic solar cells by using computational approach." *Materials Science in Semiconductor Processing* 148 (2022): 106812.
  22. Ijaz Ahmad Bhatti, Muhammad Mohsin, Nyla Amjad, **Rao Aqil Shehzad**, Khurshid Ayub, Javed Iqbal, and T. A. Taha. "Enhancement of NLO properties of supersalt (Al(BH<sub>4</sub>)<sub>3</sub>)-doped graphene: a DFT study." *Journal of Molecular Modeling* 28, no. 6 (2022): 1-15.
  23. **Rao Aqil Shehzad**, Khurshid Ayub, M. S. Al-Buriahi, Nada Alfryyan, H. H. Smaili, Sultan Alomairy, and Javed Iqbal. "Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%." *Solar Energy* 237 (2022): 96-107.
  24. Talha Ishfaq, Rasheed Ahmad Khera, Saba Zahid, Umer Yaqoob, **Rao Aqil Shehzad**, Khurshid Ayub, and Javed Iqbal. "Enhancement in nonlinear optical properties of Graphitic Carbon Nitride (C<sub>2</sub>N) by doping Superalkali (Li<sub>3</sub>O): A DFT Study." *Computational and Theoretical Chemistry* 1211 (2022): 113654.
  25. Humna Zahid, Zanib ul Ghazali, **Rao Aqil Shehzad**, Javed Iqbal, M. S. Al-Buriahi, Nada Alfryyan, Zakaria MM Mahmoud, and Z. A. Alrowaili. "Designing phenyl-di-p-tolyl-amine-based asymmetric small molecular donor materials with favorable photovoltaic parameters." *Optik* 256 (2022): 168739.
  26. Mubashar Ilyas, Ali Raza Ayu, **Rao Aqil Shehzad**, Maroof Ahmad Khan, Mehvish Perveen, Saniyah Amin, Shabbir Muhammad, and Javed Iqbal. "A DFT approach for finding therapeutic potential of two dimensional (2D) graphitic carbon nitride (GCN) as a drug delivery carrier for curcumin to treat cardiovascular diseases." *Journal of Molecular Structure* 1257 (2022): 132547.
  27. Muhammad Hussnain, **Rao Aqil Shehzad**, Shabbir Muhammad, Javed Iqbal, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, Khurshid Ayub, and Muhammad Yaseen. "Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene." *Journal of Molecular Modeling* 28, no. 2 (2022): 1-10.
  28. Naila Naeem, **Rao Aqil Shehzad**, Muhammad Ans, Mohammed Salim Akhter, and Javed Iqbal. "Dopant Free Triphenylamine-Based Hole Transport Materials with Excellent Photovoltaic Properties for High-Performance Perovskite Solar Cells." *Energy Technology* 10, no. 2 (2021): 2100838.

29. Qaba Qusain Afzal, Kinza Jaffar, Muhammad Ans, Javeria Rafique, Javed Iqbal, **Rao Aqil Shehzad**, and Muhammad Shabir Mahr. "Designing benzothiadiazole based highly efficient non-fullerene acceptor molecules for organic solar cells." *Polymer* 238 (2022): 124405.
30. Saqib Shafiq, **Rao Aqil Shehzad**, Muhammad Yaseen, Khurshid Ayub, Ali Raza Ayub, Javed Iqbal, Khaled H. Mahmoud, and Zeinhom M. El-Bahy. "DFT study of OLi3 and MgF3 doped boron nitride with enhanced nonlinear optical behavior." *Journal of Molecular Structure* 1251 (2021): 131934.
31. Rida Fatima, **Rao Aqil Shehzad**, Alvina Rasool, Muhammad Yaseen, Saleem Iqbal, Muhammad Jawwad Saif, and Javed Iqbal. "Exploring the potential of tetraazaacene derivatives as photovoltaic materials with enhanced photovoltaic parameters." *International Journal of Quantum Chemistry* 122, no. 1 (2022): e26817.
32. Naila Naeem, Tahreem Tahir, Muhammad Ans, Alvina Rasool, **Rao Aqil Shehzad**, and Javed Iqbal. "Molecular engineering strategy of naphthalimide based small donor molecules for high-performance organic solar cells." *Computational and Theoretical Chemistry* 1204 (2021): 113416.
33. Saba Zahid, Alvina Rasool, **Rao Aqil Shehzad**, Ijaz Ahmad Bhatti, and Javed Iqbal. "Tuning the optoelectronic properties of triphenylamine (TPA) based small molecules by modifying central core for photovoltaic applications." *Journal of Molecular Modeling* 27, no. 9 (2021): 1-14.
34. Alvina Rasool, Saba Zahid, **Rao Aqil Shehzad**, Muhammed Salim Akhter, and Javed Iqbal. "Designing of benzodithiophene (BDT) based non-fullerene small molecules with favorable optoelectronic properties for proficient organic solar cells." *Computational and Theoretical Chemistry* 1203 (2021): 113359.
35. Ali Raza Ayub, **Rao Aqil Shehzad**, Saleh S. Alarfaji, and Javed Iqbal. "Super alkali (OLi3) doped boron nitride with enhanced nonlinear optical behavior." *Journal of Nonlinear Optical Physics & Materials* 29, no. 01n02 (2020): 2050004.
36. **Rao Aqil Shehzad**, Shabbir Muhammad, Aijaz Rasool Chaudhry, Soichi Ito, Javed Iqbal, Muhammad Khalid, Zouhaier Aloui, and Hong-liang Xu. "Electro-optical and charge transport properties of chalcone derivatives using a dual approach from molecule to material level simulations." *Computational and Theoretical Chemistry* 1203 (2021): 113349.
37. Muhammad Ishaq, **Rao Aqil Shehzad**, Muhammad Yaseen, Saleem Iqbal, Khurshid Ayub, and Javed Iqbal. "DFT study of superhalogen-doped borophene with enhanced nonlinear optical properties." *Journal of Molecular Modeling* 27, no. 6 (2021): 1-11.
38. Qurat ul Ain, **Rao Aqil Shehzad**, Umer Yaqoob, Arooba Sharif, Zubia Sajid, Sidra Rafiq, Saleem Iqbal, Muhammad Khalid, and Javed Iqbal. "Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell." *Computational and Theoretical Chemistry* 1200 (2021): 113238.
39. **Rao Aqil Shehzad**, Shabbir Muhammad, Javed Iqbal, Abdullah G. Al-Sehemi, Muhammad Yaseen, Zouhaier Aloui, and Muhammad Khalid. "Exploring the optoelectronic and third-order nonlinear optical susceptibility of cross-shaped molecules: insights from molecule to material level." *Journal of Molecular Modeling* 27, no. 1 (2021): 1-10.
40. Asmat Ullah Khan, Rasheed Ahmad Khera, Naveed Anjum, **Rao Aqil Shehzad**, Saleem Iqbal, Khurshid Ayub, and Javed Iqbal. "DFT study of superhalogen and superalkali doped graphitic carbon nitride and its nonlinear optical properties." *RSC Advances* 11, no. 14 (2021): 7779-7789.
41. Asmat Ullah Khan, Shabbir Muhammad, Rasheed Ahmad Khera, **Rao Aqil Shehzad**, Khurshid Ayub, and Javed Iqbal. "DFT study of superhalogen (AlF4) doped boron nitride for tuning their nonlinear optical properties." *Optik* 231 (2021): 166464.
42. **Rao Aqil Shehzad**, Javed Iqbal, Muhammad Usman Khan, Riaz Hussain, Hafiz Muhammad Asif Javed, Ateeq ur Rehman, Muhammad Usman Alvi, and Muhammad Khalid. "Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells." *Computational and Theoretical Chemistry* 1181 (2020): 112833.
43. **Rao Aqil Shehzad**, Javed Iqbal, Khurshid Ayub, Faisal Nawaz, Shabbir Muhammad, Ali Raza Ayub, and Saleem Iqbal. "Enhanced linear and nonlinear optical response of superhalogen (Al7) doped graphitic carbon nitride (g-C3N4)." *Optik* 226 (2021): 165923.
44. Shabbir Muhammad, **Rao Aqil Shehzad**, Javed Iqbal, Abdullah G. Al-Sehemi, M. Saravanabhavan, and Muhammad Khalid. "Benchmark study of the linear and nonlinear optical polarizabilities in

proto-type NLO molecule of para-nitroaniline." Journal of Theoretical and Computational Chemistry 18, no. 06 (2019): 1950030.

### Combining the strengths of synthesis, chemical biology, and materials

45. Zuber a Naseem, **Rao Aqil Shehzad**, Sobia Jabeen, Suman Tahir, Farwa Mushtaq, Muhammad Zahid, and Javed Iqbal. "Quantum chemical investigation of choline chloride-based deep eutectic solvents." Chemical Physics (2023) 571: 111936.
46. Zuber a Naseem, **Rao Aqil Shehzad**, Ansum Ihsan, Javed Iqbal, Muhammad Zahid, Amjad Pervaiz, and Ghulam Sarwari. "Theoretical investigation of supramolecular hydrogen-bonded choline chloride-based deep eutectic solvents using density functional theory." Chemical Physics Letters 769 (2021): 138427.



### Certifications

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1. "Recent FE-SEM developments for material characterization: Combining Gemini optics and image processing", SelectScience, December 14, 2022.
2. "What Cleaning a Column Can Teach About HPLC Basics - EUR", eLearning Phenomenex, November 9, 2022.
3. "Pirates of Chromatography: Tales of Sharp Peaks-EUR", eLearning Phenomenex, October 31, 2022.
4. "How to seamlessly integrate the supply of purified water in new laboratory construction", SelectScience, September 27, 2022.
5. "Lowering the Energy Barrier to Great Chemistry with ChemDraw & ChemOffice", SelectScience, September 20, 2022.
6. "An overview of Preparative Chromatography - EUR", eLearning Phenomenex, August 30, 2022.
7. "Exploring LC Selectivity Using Steroids in a Clinical Setting (North America)", eLearning Phenomenex, July 26, 2022.
8. "Broadband benchtop NMR spectroscopy: it's more than just protons", Chemistry World Webinars, June 29, 2022.
9. "Introduction to EDS Large Area Mapping in SEM", Oxford Instruments, June 23, 2022.
10. "Fingerprinting recycled thermoplastic resins for process optimization", Chemistry World Webinars, June 15, 2022.
11. "Empowering ethical knowledge publishing: Mastering art identifying predatory fake, cloned journals", Presented by Vishal Gupta, Senior Customer Consultant-Elsevier, Prof. Sumit Narula Deputy Dean (Research & Publications)-Amity University Gwalior, June 8, 2022.
12. "Shine a light on your chemistry with in-situ photo-NMR", Chemistry World Webinars, March 30, 2022.
13. "Driving the development of bio-based polymers with molecular simulation", Chemistry World Webinars, April 13, 2022.
14. "The Universal HPTLC Mix (UHM): A new concept for System Suitability Tests (SST) in high-performance thin-layer chromatography", SelectScience, June 4, 2022.
15. "RSC Desktop Seminar - Hosted by Environmental Science: Advances", RSC Publishing Webinars, June 1, 2022.
16. "Rapid Methods and Automation in Food Microbiology: Developments, Promise and Challenges", Willey Analytical Science, April 26, 2022.
17. "Characterization of Optical Layers Using UV-Vis / NIR Spectroscopy", Willey Analytical Science, April 28, 2022.
18. "RSC-IISER Desktop Seminar with Dalton Transactions", RSC Publishing Webinars, May 12, 2022.
19. "Belonging and connection - Building a better chemistry culture", Chemistry World Webinars, May 10, 2022.
20. "Unique GC Column Selectivities for Optimal Separation of PAH Compounds in Food and Environmental Matrices", SelectScience, May 10, 2022.
21. "Size-exclusion chromatography: How to upgrade your current methods", SelectScience, April 20, 2022.

22. "Shine a light on your chemistry with in-situ photo-NMR", Chemistry World Webinars, March 30, 2022.
23. "UHPLC: Level up your method transfer and scaling", SelectScience, March 29, 2022.
24. "Level up your nanoparticle quant and sizing on Stunner", SelectScience, March 10, 2022.
25. "Powerful technology through tiny particles: Innovation with aqueous colloidal silica", Chemistry World Webinars, February 22, 2022.
26. "Centrifugal partition chromatography: Isolation of mono-aromatic compounds from oxidatively depolymerized lignin", SelectScience, February 23, 2022.
27. "In situ material testing in SEM: Achieve an unprecedented level of automation", SelectScience, February 17, 2022.
28. "Using flow chemistry to give early drug discovery processes a boost", RSC Publishing Webinars, January 26, 2022.
29. "Substitution of hazardous substances: Top tips to minimizing exposure and complying with legislation", SelectScience, January 18, 2022.
30. "Promoting Research Excellence Academics Across Pakistan", Higher Education Commission, Pakistan, Feb 1-2, 2022.
31. "RSC Desktop Seminar Series with RSC Medicinal Chemistry & RSC-BMCS", RSC Publishing Webinars, January 12, 2022.
32. "Identification of protein aggregation through UV-Visible spectroscopy: The use of absorption and diffuse reflection techniques", SelectScience, January 26, 2022.
33. "Advanced techniques in SEM and EDS for biological samples", SelectScience, January 26, 2022.
34. "Clinical research analysis of perfluoroalkyl substances (PFASs) in human serum by LC-MS/MS using Captiva EMR-Lipid cleanup", SelectScience, January 20, 2022.
35. "A multi-platform metabolomics approach for exposure science using mass spectrometry", SelectScience, December 16, 2021.
36. "RSC Desktop Seminar Series with RSC Medicinal Chemistry & RSC-BMCS", RSC Publishing Webinars, December 9, 2021.
37. "RSC Desktop Seminar Series with RSC Medicinal Chemistry & RSC-BMCS", RSC Publishing Webinars, December 8, 2021.
38. "Efficient modelling of polymers for industrial applications using molecular dynamics", Chemistry World Webinars, December 9, 2021.
39. "A masterclass in multiplex immuno-fluorescent image analysis of tumor samples", SelectScience, December 15, 2021.
40. "Utilizing new and unique GC column selectivities for optimal separation of dioxins, PCBs, and PAHs in environmental and food matrices", SelectScience, December 8, 2021.
41. "Simplify your life in the lab: Explore the power of Precellys for your DNA and RNA workflows", SelectScience, December 2, 2021.
42. "RSC-IISER Desktop Seminar with OBC", Chemistry World Webinars, November 25, 2021.
43. "How a private testing lab realigned its services to meet the needs of the global pandemic", SelectScience, November 29, 2021.
44. "Taking chemistry to market", Chemistry World Webinars, November 23, 2021.
45. "Integrated volume verification: Providing a safety net for your liquid handling workflows", SelectScience, November 24, 2021.
46. "Separating polar analyte mixtures: Benefits of a new zwitterionic HILIC chemistry", SelectScience, November 24, 2021.
47. "Ensuring accuracy: An expert guide to selecting fit-for-purpose reference materials", SelectScience, November 24, 2021.
48. "Optimizing protein stability using new computational design approaches for biologics", Chemistry World Webinars, November 18, 2021.
49. "Optimizing battery performance through materials characterization", Chemistry World Webinars, November 10, 2021.
50. "Laser-induced breakdown spectroscopy quantification: From fundamental understanding to data processing", SelectScience, November 12, 2021.
51. "An automated purification workflow to ensure drinking water purity and safety", SelectScience, November 10, 2021.
52. "Monitoring electronic excitations in organic semiconductors with ultrafast optical pump-probe spectroscopy", SelectScience, November 8, 2021.
53. "Taking your first steps towards automation: Simple, intuitive, and affordable liquid handling", SelectScience, November 8, 2021.

54. "Volumetric titration: A step-by-step guide to correct results", SelectScience, November 8, 2021.
55. "Become a Drug Testing Wiz with MS  $\beta$ -glucuronidases: Simplify your urinolysis workflow", SelectScience, November 8, 2021.
56. "Sublime precursors: how modelling organometallics at surfaces drives innovation in materials processing" Chemistry World Webinars, October 28, 2021.
57. "RSC-IISER Desktop Seminar with ChemComm", RSC Publishing Webinars, August 6, 2021.
58. "Novel Electron Detection and Imaging Strategies in SEM for Enhanced Quantification of Second Phases", ThermoFisher Scientific, January 11, 2022.
59. "Online training workshop on Computational Density Functional Theory", Thanthai Periyar Government Polytechnic College Vellore -632 002, Tamil Nadu, India, Jul 4-5, 2020.
60. "e-Roozgar in the Technical Course", August 10 to November 9, 2020, Batch 3, University of Okara.
61. "Docking, QSAR and Molecular Dynamics" Department of Biotechnology, Ramaiah Institute of Technology and Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ramaiah University of Applied Sciences, Bengaluru, Karnataka, India in association with IEEE-EMB MSRIT student chapter and SRIGEN-Society of Biotechnologists from July 29 to 31, 2020.
62. "Excellent performance and contribution in curricular & extracurricular activities in the Department of Chemistry", University of Okara, Session 2014-2018.
63. "One-day International Online Symposium on Recent Trends in Chemistry", Department of Chemistry, University of Okara, September 10, 2020.
64. "How to Utilize ProQuest eBooks Collection in Teaching and Research" on Tuesday, October 20, 2020, in partnership with Higher Education Commission (HEC).
65. "How to Manage Your References Using RefWorks" on Tuesday, December 1, 2020, in partnership with Higher Education Commission (HEC).
66. "Environmental Science: Atmospheres RSC Desktop Seminar featuring our inaugural authors", RSC Publishing Webinars, April 21, 2021.
67. "Global Trends in Combating Environmental and Agricultural Issues", Department of Environmental Sciences, University of Okara, September 23, 2021.
68. "Li-ion battery electrolyte degradation characterization by mass spectrometry", Chemistry World Webinars, June 8, 2021.
69. "A recipe for success in exploiting machine learning and data science", Chemistry World Webinars, June 15, 2021.
70. "Quantitative structural analysis using STEP HAADF-iDPC", Chemistry World Webinars, July 12, 2021.
71. "Reviewing manuscripts in the 2<sup>nd</sup> iiScience Int'l Conference 2021 held as an Online Event", jointly organized by GC Women University, Faisalabad, Pakistan, with the partnership of UNC Charlotte, North Carolina, USA and with the Technical Sponsorship by the SPIE, March 29-30, 2021.
72. "The age of digital chemistry", Chemistry World Webinars, June 29, 2021.
73. "Portable Spectroscopy: Field, Industrial and Anti-Counterfeiting Applications", Wiley Team, July 22, 2021.
74. "Trends in modern hit discovery: How your ultra-large screens can benefit from machine learning", Chemistry World Webinars, July 29, 2021.
75. "Discover the possibilities with the new multi-sample Discovery X3 Differential Scanning Calorimeter", Chemistry World Webinars, September 2, 2021.





## Computational Experience

◆ Material Studio	◆ GaussView	◆ Gaussian
◆ OriginPro	◆ Microsoft Office	◆ Swizard
◆ PyMOlyze	◆ Multiwfn	◆ Linux OS
◆ Windows OS	◆ Software and Hardware	◆ AOMix
◆ Avogadro	◆ ChemOffice	◆ Mercury
◆ VMware	◆ EndNote	◆ WordPress
◆ MATLAB	◆ MiniTab	◆ VirtualBox
◆ Mendeley	◆ VEDA	◆ Match
◆ CASTEP	◆ Crystal Explorer	◆ VMD
◆ ChemCarft	◆ SCOPS	◆ Filmora
◆ Adobe Photoshop	◆ Adobe Illustrator	



## References

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