Zakir Ullah

Institute De Ciencia De Materials De Barcelona (ICMAB-CSIC), Spain.

+34-634251100, zullah@icmab.es , azazay1@gmail.com

Google Scholar , ORCID: 0000-0001-8647-1986

Research Interests: Synthetic and Computational Chemistry, Energy Storage, Photoswitching, UV-Vis Spectroscopy, IR Spectroscopy, Electronic Structures Simulations, Sensors Synthesis, Sensors Simulations, Porous Organic Network for Sensor, Adsorption, CO_2 Catalysis, Organometallic Reaction Mechanism by Using DFT, Theoretical Simulations for Chemical Reactions, Solar cells.

Education and Research Experience

Institute De Ciencia De Materials De Barcelona
(ICMAB-CSIC), Spain) March 2023 –to- date
Juan de la Cierva fellowship
Project: Sustainable Energy Conversion and Storage Systems.
Advisor: **Prof**. David Brian Amabilino

Incheon National University (INU), South Korea Sept 2021 – Feb 2023
Post-doctorate
Project: Design and Synthesis of Sensor for Insect Vector diseases
Advisor: **Prof**. Hyung Wook Kwon

Korea Advanced Institute of Science and Technology (KAIST), South Korea Sept 2016–Aug 2021
Doctoral Program (Ph.D. in Chemistry)
Thesis Title: Design and Synthesis of Multifunctional molecules and
Porous Organic Networks for Sensor, Adsorption, and Catalysis:
A Combined Experimental and DFT Study.
Advisors: **Prof**. David G. Churchill, **Prof**. Mu-Hyun Baik, and **Prof**. Cafer T. Yavuz.

Gachon University, South Korea March 2015–Aug 2016
Doctoral Program and later move to KAIST
Project: Experimental and DFT Study of Green Catalyst Designing for Organic Synthesis
Advisor: **Prof**. Mihyun Kim

University of Peshawar (UOP), Pakistan Sept 2012–Feb 2015
M.Phil. Chemistry
Project: Density Functional Theory and Experimental Study of Diospyrin and 8-hydroxydiospyrin
Advisor: **Prof**. Atta-ur-Rahman and **Prof**. Khurshid Ayub

Kohat University of Science and Technology (KUST), Pakistan
MSc. Chemistry
Project: Antibacterial study of Phyla nodiflora Linn Sept 2008–March 2011
Advisor: **Prof**. Ijaz Ahmed

University of Peshawar (UOP), Pakistan
B.Sc. Biological Science (Chemistry and Biology) Sept 2006 – Sept 2008

Research Articles:

In Preparation / Submitted / Under Review

61. "Two-dimensional porous MXene@C2N heterostructures for HER", In preparation for Advanced Energy (**Equal First Author**)

60. "A "Catch Toy"-like Motif: DFT and SERS Study of Nanocage Adsorption in the Concave Side of a Biscorrole and Porphyrin-host Valency" Youngseob Lee, Zakir Ullah, Donghyeon Kim, Sheena Mary, Hyung Wook Kwon, Kyung-Bin Cho, and David G. Churchill, In preparation for *Surface and Interfaces* (**Equal First Author**)

59. "Fe/Fe3C Embedded Pyrazine-Based Porous Organic Network for Superior Tribo-charge and Electrochemical Double Layer Capacitance" Muhammad Noman, Qazi Muhammad Saqib, Ishfaq Ahmad, Zakir Ullah, Cafer T. Yavuz, and Jinho Bae, to be submitted to Advanced Energy (**Corresponding Author**)

58. "Unlocking water coordination environment in Co-based Metal-Organic Frameworks for advanced Nitrate-to-Ammonia Electroreduction" Muthukumar, Pandi; Ullah, Zakir; Zhang, Xia; Ullah, Habib; Liu, Yuxiao ; Li, Linfeng; Zhou, Xianlong; Anthony, Savarimuthu; Zuo, Yunpeng; Wang, Xin; Wang, Chundong, Submitted to JACS (**Equal First Author**)

57. "Layered Arrangement of Polyoxometalate on Metal-Organic Framework as a High-Capacity Anode Material for Sodium-ion Batteries." Ullah, Irfan; Aldhafeeri, Tahani; Haider, Ali; Wu, Xianyong ; Ullah, Zakir; Chang, Songyang; Inayat, Abid; bibi, Nosheen; Pope , Michael; Sher, Falak; Rehman, Habib ur; Hussain, Irshad. ACS Applied Energy Materials, (**Online**) https://doi.org/10.1021/acsaem.4c02904 **Q1, IF = 5.5, Co-Author**)

56. "Solvent Free Ambient Pressure CO2 Cycloaddition Catalyzed by Cobalt-Impregnated 2D-Nanofibrous COFs" Habib Ullah, Zakir Ullah, Bibi Maryam Mousavi, Hussain A. Younus, Zafar A. K. Khattat, Suleman Suleman, Hossain M. Shahadat, Baoyi Yu, Hyun You Kim, and Francis Verpoort,; *ChemSuschem* **(Online)** https://doi.org/10.1002/cssc.202401046 **Q1, IF = 8.4, Corresponding Author**)

Published

55. "High-Efficiency Triple-Junction Polymer Solar Cell: A Theoretical Approach" Fazli Sattar, Xiaozhuang Zhou and Zakir Ullah,; Molecules ***2024***, *29(22), 5370*. https://doi.org/10.3390/molecules29225370 (**Q1, IF = 4.2, Corresponding Author**)

54. "Corrole-Chelated Metal Complexes Enabling Dual C-H Chlorination and H_2O_2 Generation" Xuan Zhan, Donghyeno Kim, Zakir Ullah, and David G. Churchill. *Journal of Molecular Liquids 413 (**2024**) 125938.* https://doi.org/10.1016/j.molliq.2024.125938 (**Q1, IF = 5.3, Corresponding Author**)

53. "Amplifying High-Performance Organic Solar Cells through Differencing Interactions of Solid Additive with Donor/Acceptor Materials Processed from Non-Halogenated Solvent" has been received by journal Advanced Energy Materials" Muhammad Haris, Zakir Ullah, Seungjin Lee, Du Hyeon Ryu, Seung Un Ryu, Bong Joo Kang, Nam Joong Jeon, Bumjoon J. Kim, Taiho Park, Won Suk Shin, and Chang Eun Song. *Adv. Energy Mater.* ***2024***, *2401597. https://doi.org/10.1002/aenm.202401597* (**Q1, IF = 24.4, Equal First Author**)

52. "Battling Hazardous Gas Molecules with Kekulene Surfaces: A Computational Study". Fazli Sattar, Zhenzhen Wang, Xiozhuang Zhou, and Zakir Ullah* *Journal of Molecular Liquids (**2024**): 125099.* https://doi.org/10.1016/j.molliq.2024.125099 (**Q1, IF = 5.3, Corresponding Author**)

51. "Exploring Nitric Acid's Role in Photo-Catalytic Conversion: Synergy with Phosphorus Corrole for Enhanced Mesitylene Transformation". Xuan Zhan and Zakir Ullah; *Journal of Molecular Catalysis (***2024***)* https://doi.org/10.1016/j.mcat.2024.114229 (**Q2, IF = 3.9, Corresponding Author**)

50. "Methotrexate-loaded Fe-metal organic frameworks: Synthesis, characterizations, drug release investigations". Uzma Yunus, Muhammad Ejaz Khan, Saiqa Sadiq, Muhammad Aamir, Zakir Ullah, Moazzam H. Bhatti, Mohammad Sher and Gul-e-Saba Chaudhry; *Journal of Drug Delivery Science and Technology* (**2024**) https://doi.org/10.1016/j.jddst.2024.105790 (**Q1, IF = 4.5, Co-Author**)

49. "Hydrogen-bonding interactions between terpolymers enable excellent device efficiency and operational stability of non-halogenated solvent-processed polymer solar cells" Fiza Arshad, Muhammad Haris, Eun Sung Oh, Zakir Ullah, Du Hyeon Ryu, Seungjin Lee, Hang Ken Lee, Sang Kyu Lee, Taek-Soo Kim, Hyung-Wook Kwon, Chang Eun Song, Won Suk Shin. *AdFM* (**2024**) https://doi.org/10.1002/adfm.202402045 (**Q1, IF = 16, Equal First Author**)

48. "Unlocking potential diabetes therapeutics: Insights into alpha-glucosidase inhibition", Saima Malik, Muhammad Arif Lodhi, Sultan Ayaz, Zakir Ullah, *Journal of Molecular Liquids*. (**2024)** https://doi.org/10.1016/j.molliq.2024.124572 **Q1, IF = 6.0, Corresponding Author**)

47. "Highly selective and scalable molecular fluoride sensor for naked-eye detection" Zakir Ullah, Saravanan Subramanian, Haeseong Lim, Nesibe A Dogan, Joo Sung Lee, Thien S Nguyen, Cafer T Yavuz, *ACS Applied Materials & Interfaces* (**2024**) https://doi.org/10.1021/acsami.4c01187 (**Q1, IF = 9.5, First Author**)

46. "Morphological modulation enabled by non-halogenatedsolvent-processed simple solid additives for high-efficiencyorganic solar cells" Muhammad Haris, Du Hyeon Ryu, Zakir Ullah, Bong Joo Kang, Nam Joong Jeon, Seungjin Lee, Hang Ken Lee, Sang Kyu Lee, Jong-Cheol Lee, Hyung-Wook Kwon, Won Suk Shin, and Chang Eun Song. *EcoMat* (**2024**) https://doi.org/10.1002/eom2.12436 (**Q1, IF = 12.21, Equal First Author**)

45. "Photophysics of corroles and closely related systems for emergent solar energy, medicinal, and materials science applications" Xuan Zhan, Donghyeon Kim, Zakir Ullah, Woohyun Lee, Zeev Gross, David G. Churchill. *Coord. Chem. Rev.* (**2023**) https://doi.org/10.1016/j.ccr.2023.215363 (**Q1, IF = 24.83, Equal First Author**)

44. "Porous Organic Cages". Xinchun Yang, Zakir Ullah, J. Fraser Stoddart, Cafer T. Yavuz. ACS Chemical Review. (**2023**) https://doi.org/10.1021/acs.chemrev.2c00667 **Q1, IF = 72, Equal First Author**)

43. "*Unlocking the potential of ovalene: A dual-purpose sensor and drug enhancer*" Zakir Ullah, Hyun Jee Kim, Y Sheena Mary, Naseer Belboukhari, Khaled Sekkoum, Aicha Kraimi, Xuan Zhan, Hyung Wook Kwon. *Journal of Molecular Liquids*. (**2023)** https://doi.org/10.1016/j.molliq.2023.121540 **Q1, IF = 5.3, First and Corresponding Author**)

42. "*Substituent Effect on Ligand-Centered Electrocatalytic Hydrogen Evolution of Phosphorus Corroles*" Gang Yang, Zakir Ullah, Wu Yang, Hyung Wook Kwon, Zhen-Xing Liang, Xuan Zhan, Gao-Qing Yuan, Hai-Yang Liu. *ChemSusChem*. (**2023**) https://doi.org/10.1002/cssc.202300211 **Q1, IF = 8.47, Corresponding Author**)

41. "*Formation of Value-Added Cyclic Carbonates by Coupling of Epoxides and CO2by Ruthenium Pincer Hydrazone Complexes under Atmospheric Pressure*" Habib Ullah, Zakir Ullah, Zafar A. K. Khattak, Mohsin Ali Marwat, Baoyi Yu, Hyung Wook Kwon, Hyun You Kim, and FrancisVerpoort. *ACS Energy&Fuels* (**2023**) https://doi.org/10.1021/acs.energyfuels.2c03611 **Q1, IF = 4.65, Equal firts Author**)

40. "*DFT, solvation effects, reactivity and SERS analysis on structural, optical, and vibrational properties of a biomolecule of pyrimidine derivative adsorbed on metal clusters of Ag/Au/Cu*" Jamelah S Al-Otaibi, Y Sheena Mary, Y Shyma Mary, Nivedita Acharjee, Zakir Ullah. *Journal of the Indian Chemical Society*. (**2022)** https://doi.org/10.1016/j.jics.2022.100753 **Co-Author)**

39. "Nutrition for Honey Bee to Prevent Colony Collapse" Hyun Jee Kim, Gyu Been Seo, Zakir Ullah, and Hyung Wook Kwon. *Journal of Apiculture*. (**2022**) DOI: 10.17519/apiculture.2022.11.37.4.397 **Co-Author**)

38. "*Adsorption of Pyrimidine-2-amine(PA) on Graphene Quantum Dots(GQDs): Non-covalent Interaction Study*" Zakir Ullah, Y Sheena Mary, Hyun Jee Kim, and Hyung Wook Kwon. *Journal of Molecular Liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.120654 **Q1, IF = 5.3, First and Corresponding Author**)

37. "Insight into *Caffeine Adsorption on the Surface of Corannulene: A sensor Study*" Zakir Ullah, Y Sheena Mary, Hyun Jee Kim, and Hyung Wook Kwon. *Journal of Molecular Liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.120592 **Q1, IF = 5.3, First and Corresponding Author**)

36. "*Computational Study of Toxic Gas Removal*" Zakir Ullah, Fazli Sattar, Hyun Jee Kim, Sooin Jang, Y. Sheena Mary, Xuan Zhan, and Hyung Wook Kwon. *Journal of Molecular Liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.120213 (**Q1, IF = 5.3, First and Corresponding Author**)

35. "*Computational Study of Pd–Cd Bimetallic Crystals: Spectroscopic Properties, Hirshfeld surface analysis, Non-Covalent Interaction, and Sensor Activity*" Zakir Ullah, Fazli Sattar, Hyun Jee Kim, Sooin Jang, Y. Sheena Mary, Xuan Zhan, and Hyung Wook Kwon. *Journal of Molecular liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.120111 (**Q1, IF = 5.3, First and Corresponding Author**)

34. "*Comparison of physicochemical properties of pollen substitute diet for honey bee (Apis mellifera)*" Hyun Jee Kim, Jinseok Hwang, Zakir Ullah, Bilal Mustafa, Hyung Wook Kwon. *Journal of Asia-Pacific Entomology*. (**2022**) https://doi.org/10.1016/j.aspen.2022.101967 (**Q2, IF = 1.30, co-author)**

33. "*Computational Study of Furosemide-Piperazine (FS–PZ) and 2, 3, 5, 6-tetramethylpyrazine (FS-TP) Co-Crystals*" Zakir Ullah, Jamelah S Al-Otaibi, Y Sheena Mary, Hyung Wook Kwon. *Journal of Molecular liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.119537 (**Q1, IF = 5.3, First and Corresponding Author**)

32. "*Adsorption of Diospyrin on the Surface of CC/AlN/AlP/GaN Nanotubes: A DFT Investigation*" Zakir Ullah, Xuan Zhan, Sooin Jang, Hyun Jee Kim, Y Sheena Mary, Jamelah S Al-Otaibi, Hyung Wook Kwon. *Journal of Molecular liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.119472 (**Q1, IF = 5.3, First and Corresponding Author**)

31. "*DFT Study of 6-amino-3-(1-hydroxyethyl) pyridine-2, 4-diol (AHP) Adsorption on Coronene*" Zakir Ullah, Hyun Jee Kim, Sooin Jang, Y Sheena Mary, Hyung Wook Kwon. *Journal of Molecular liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.119436 (**Q1, IF = 5.3, First and Corresponding Author**)

30. "*DFT investigations on conformational analysis, solvation effects, reactivity studies, chemical descriptors and docking of two anti-cancerous drugs, Lenvatinib and Regorafenib*" Jamelah S Al-Otaibi, Zakir Ullah, Y Sheena Mary, Y Shyma Mary, Sreejit Soman, M Thirunavukkarasu, Hyung Wook Kwon. *Vietnam J. Chem., **2022**, 60(5), 636-652*. (**2022**) https://doi.org/10.1002/vjch.202200013

29. "*β-Bis-CF 3-substituted phosphorus corroles, theory and experiments*" Xuan Zhan, Zakir Ullah, Dong Hyeon Kim, Bilal Mustafa, Hyungwook Kwon, David G Churchill, Zeev Gross. *Inorganic.Chemistry.Frontier.* (**2022**) https://doi.org/10.1039/D1QI01620B (**Q1, IF = 7.77, Equal first author)**)

28. "*Selective Detection of F– ion and SO2, Solvent effect, Molecular Docking, and Mechanistic Study*" Zakir Ullah A Kraimi, HJ Kim, S Jang, YS Mary, HW Kwon. *Journal of Molecular liquids*. (**2022**) https://doi.org/10.1016/j.molliq.2022.119329 (**Q1, IF = 5.3, First and Corresponding Author**)

27. "*DFT of 5-Fluoro-2-Oxo-1H-Pyrazine-3-Carboxamide (OPC) Adsorption, Spectroscopic, Solvent Effect, and SERS Analysis*". Zakir Ullah, Bilal Mustafa, Hyun Jee Kim, Y. Sheena Mary, Y. Shyma Mary, and Hyung Wook Kwon. *Journal of Molecular Liquids* (**2022**). https://doi.org/10.1016/j.molliq.2022.119076 (**Q1, IF = 5.3, First and Corresponding Author**)

26. "*A foundational theoretical Al12E12 (E = N, P) adsorption and docking study: cage–quinolone pairs, optics, and possible therapeutic and diagnostic applications*". Zakir Ullah, Prasad M. Sonawane, Y. Sheena Mary, C. Yohannan Panicker, and David G. Churchill. *J. Biomol. Struct. Dyn.* (**2022**) https://doi.org/10.1080/07391102.2022.2053742 (**Q2, IF = 4.15, First Author**)

25. "*Adsorption behavior and solvent effects of an adamantane-triazolederivative on metal clusters – DFT simulation studies*". amelah S. Al-Otaibi, Y. Sheena Mary, Y. Shyma Mary, Zakir Ullah, Hyung Wook Kwon; *Journal of Molecular Liquids* 345 (**2022**) 118242. https://doi.org/10.1016/j.saa.2021.120677 **(Q1, IF = 5.3)**

24. "*CCDC 1996618: Experimental Crystal Structure Determination : 1,1'-(naphthalene-1,5-diyl)bis(3-methyl-5-phenyl-1H-pyrazole)*" Mousumi Garai, Manmatha Mahato, Yeongran Hong, Vepa Rozyyev, Uiseok Jeong, Zakir Ullah, Cafer T Yavuz. (**2021**) http://hdl.handle.net/10754/686922 Co-**Author)**

23. "*Adsorption properties of dacarbazine with graphene/fullerene/metal nanocages – Reactivity, spectroscopic and SERS analysis*". Jamelah S. Al-Otaibi, Y. Sheena Mary, Y. Shyma Mary, Zakir Ullah, Rohitash Yadav, Nitin Gupta David G. Churchill; *Spectrochimica Acta Part A*. **2021**. https://doi.org/10.1016/j.saa.2021.120677 **(Q1, IF = 4.47, co-author)**

22. "*Theoretical model study of adsorbed antimalarial-graphene dimers: doping effects, photophysical parameters, intermolecular interactions, edge adsorption, and SERS*". Zakir Ullah, Prasad M Sonawane, Y Sheena Mary, Y Shyma Mary, Pratap Mane, Brahmananda Chakraborty, David G Churchill; *J. Biomol. Struct. Dyn*, **2021**, https://doi.org/10.1080/07391102.2021.1990129 (**Q2, IF = 4.15, First Author**)

21. "*LBL generated fire retardant nanocomposites on cotton fabric using cationized starch-clay-nanoparticles matrix*". Zeeshan Ur Rahman, Seok-Hwan Huh, Zakir Ullah, Ye-Tang Pan, David G Churchill, Bon Heun Koo; *Carbohydrate Polymers*, 274 (**2021**) 118626. https://doi.org/10.1016/j.carbpol.2021.118626 **(Q1, IF = 9.38)**

20. "*Computational Study of Sorbic Acid Drug Adsorption onto Coronene/Fullerene/Fullerene-Like X12Y12 (X = Al, B, and Y = N, P) Nanocages*: DFT and Molecular Docking Investigations". Y. S. Mary, Y. S. Mary, Z. Ullah, *J. Cluster Sci*, **2021**, https://doi.org/10.1007/s10876-021-02106-4 (**Q2, IF = 3.06**)

19. "*Plausible pnicogen bonding of epi-Cinchonidine as a chiral scaffold in catalysis*". Z. Ullah, K. Kim, A. Venkanna, M. I. Kim, M.-h. Kim, *Front. Chem*, **2021**, 9, 481. https://doi.org/10.3389/fchem.2021.669515 **(Q1, IF = 5.54, First Author)**

18. "*Bisphenol–based cyanide sensing: selectivity, reversibility, facile synthesis, bilateral "OFF-ON" fluorescence, C_{2v} structural and conformational analysis*" Zakir Ullah, Sonawane Prasad Malhari, Thien S. Nguyen, Mousumi Gara, David G. Churchill, Cafer T. Yavuz.. *Spectrochimica Acta Part A*. **2021**, 119881. https://doi.org/10.1016/j.saa.2021.119881 **(Q1, IF = 4.47, First author)**

17. "*Asynchronous double Schiff base formation of pyrazole porous polymers for selective Pd recovery".* M. Garai, M. Mahato, Y. Hong, V. Rozyyev, U. Jeong, Z. Ullah, C. T. Yavuz, *Adv. Sci*. **2021**; 2001676. https://doi.org/10.1002/advs.202001676 **(Q1, IF = 17.52, co-author)**

16. "*Markovnikov versus anti-Markovnikov addition and C–H activation: Pd–Cu synergistic catalysis*". Zakir Ullah and Renjith, *Appl Organometal Chem*. **2021** https://doi.org/10.1002/aoc.607 **(Q1, IF = 3.77, First Author)**

15. "*Mechanistic insights can resolve the low reactivity and selectivity issues in intermolecular Rauhut–Currier (RC) reaction of γ-hydroxyenone*". Zakir Ullah and Renjith, *New J. Chem*., **2020**, 44, 12857-12865. https://doi.org/10.1039/D0NJ02732D (**Q1, IF = 3.92, First Auhtor)**

14. "*Syntheses, characterizations, crystal structures, DFT/TD-DFT, luminescence behaviors and cytotoxic effect of bicompartmental Zn (II) -dicyanamide Schiff base coordination polymers: An approach to apoptosis, autophagy and necrosis type classical cell death*". Dhrubajyoti Majumdar, Yashika Agrawal, Renjith Thomas, Zakir Ullah, Manas K Santra, Sourav Das, Tapan K Pal, Kalipada Bankura, Dipankar Mishra, *Appl Organometal Chem*. **2020**; https://doi.org/10.1002/aoc.5269 (**Q1, IF = 3.77, Co-Author)**

13. "*External stimulus controlled recombination of hydrogen in photochromic dithienylethene frustrated lewis pairs*". Fazl-i-Sattar, Arsalan Ahmad, Habib Ullah, Zakir Ullah, Muhammad Tariq, and Khurshid Ayub, *Int. J. Hydrogen Energy*. **2019.** https://doi.org/10.1016/j.ijhydene.2019.10.051 (**Q1, IF = 5.81, Co-Author)**

12. **"***Zwitterion π–conjugated network polymer based on guanidinium and β-ketoenol as a heterogeneous organo-catalyst for chemical fixation of CO2 into cyclic carbonates*". Mousumi Garai, Vepa Rozyyev, Zakir Ullah, Aqil Jamal, Cafer T Yavuz, *APL Mater*. (**2019**) https://doi.org/10.1063/1.5122017 (**Q1, IF = 6.63, Co-Author)**

11. "*Positive shift in corrole redox potentials leveraged by modest β-CF3-substitution helps achieve efficient photocatalytic CH bond functionalization for group 13 complexes*". Xuan Zhan, Pinky Yadav, Yael Diskin-Posner, Natalia Fridman, Mahesh Sundararajan, Zakir Ullah, Qiu-Cheng Chen, Linda JW Shimon, Atif Mahammed, David G Churchill, Mu-Hyun Baik, Zeev Gross, *Dalton Trans*., **2019**, https://doi.org/10.1039/C9DT02150G (**Q1, IF = 4.39, Co-Author)**

10. "*Syntheses, X-ray crystal structures of two new Zn(II)-dicyanamide complexes derived from H2vanen- type compartmental ligands: Investigation of thermal, photoluminescence, in Vitro cutotoxic effect and DFT- TDDFT studies*". Dhrubajyoti Majumdar, SouravDas, Zakir Ullah, S.S.Sreejith, Dhiraj Das, Kalipada Bankura and Dipankar Mishra, *Inorganica Chimica Acta* (**2019**) https://doi.org/10.1016/j.ica.2019.04.041 (**Q2, IF = 2.54, Co-Author)**.

9. "*Maximizing property Tuning of Phosphorous Corroles Photocatalyst through a Trifluoromethylatin Approach*". Xuan Zhan, Peter Teplitzky, Yael Diskin-Posner, Mahesh Sundararajan, Zakir Ullah, Qiu-Cheng Chen, Linda J. W. Shimon, Irena Saltsman, Atif Mahammed, Monica Kosa, Mu-Hyun Baik, David G. Churchill, Zeev Gross. *Inorg. Chem*. **2019**, https://doi.org/10.1021/acs.inorgchem.9b00436 **(Q1, IF = 5.16, Co-Author**)

8. "*Catalytic Asymmetric DearomatizationbyVisible-Light-Activated [2+2] Photocycloaddition.*" Naifu Hu, Hoimin Jung, Yu Zheng, Juhyeong Lee, Lilu Zhang, Zakir Ullah, Xiulan Xie, Klaus Harms, Mu-Hyun Baik, and Eric Meggers, *Angew. Chem. Int. Ed*. **2018**, https://doi.org/10.1002/anie.201802891 (**Q1, IF = 16.82, Co-Author)**

7. "*Metal-Free α-C (sp3)–H Functionalized Oxidative Cyclization of Tertiary N, N-Diaryl Amino Alcohols: Theoretical Approach for Mechanistic Pathway".* Zakir Ullah and Mi-Hyun Kim, *Molecules* **2017**, https://doi.org/10.3390/molecules22040547 (**Q1, IF = 5.06, First Author**).

6. "*Density functional theory and phytochemical study of 8-hydroxyisodiospyrin*." Zakir Ullah, Ata- ur-Rahman, Fazl-i-Sattar, Abdur Rauf, and Habib Ullah, *J. Molecular Structure* **2015**, https://doi.org/10.1016/j.molstruc.2015.04.027 (**Q2, IF = 3.19, First Author)**.

5. "*Phytochemical, spectroscopic and density functional theory study of Diospyrin, and non-bonding interactions of Diospyrin with atmospheric gases*." Fazl-i-Sattar, Zakir Ullah, Abdur Rauf, and Habib Ullah, *Spectrochim. Acta A* **2015**, https://doi.org/10.1016/j.saa.2015.01.022 (**Q1, IF = 4.47, co-author).**

4. "*Density Functional Theory and Phytochemical Study of Pistagremic Acid*" Habib Ullah*, Abdur Rauf, Zakir Ullah, Anwar ul Haq Ali Shah, Khurshid Ayub, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 118 (**2014**) 210–214,* https://doi.org/10.1016/j.saa.2013.08.099 (**Q1, IF = 4.47, co-author**).

3. "*Theoretical Insight of Polypyrrole as Ammonia Gas Sensor*." Habib Ullah, Khurshid Ayub*, Zakir Ullah, Muhammad Hanif, Anwar-ul-Haq Ali Shah, Salma Bilal, *Synthetic Metals 172 (**2013**) 14–20*, https://doi.org/10.1016/j.synthmet.2013.03.021 (**Q1, IF = 3.37, co-author**).

2. "*Antibacterial study of Phyla nodiflora Linn*". Zakir Ullah, Ali Rehman, Najeeb Ullah, Shakeel Ahmad Khan, Shahid Ullah Khan, and Ijaz Ahmad, *Chem. Pharm. Res*., **2013**, 5(3):86-90. (**Q3, First author**).

1. "Standardization of Eclipta alba (L)" M.Shabeer, G.A.Khan. Zakir Ullah, Akhtar Ali, *Asian J. Res. Chem.* **2011**, *4*, 1825. (**Q3, Co-author**).

Posters and Conferences:

1. **Zakir Ullah.** Int. Conference of the Korean Society for Molecular and Cellular Biology, South Korea, **2015**.
2. **Zakir Ullah**. **OMCOS 19**, Jeju South Korea **2017**. "Computational Insight into Intermolecular Rauhut Currier (RC) Reaction of γ-Hydroxyenone"
3. **Zakir Ullah**, **IBS-KAIST 2018 "**Catalytic Asymmetric Dearomatization by Visible- Light-Activated [2+2] Photocycloaddition**"**
4. **Zakir Ullah**, "Markovnikov versus anti-Markovnikov addition and C–H activation: Pd–Cu synergistic catalysis" Korean Chemical Society, **KCS 2018**.
5. **Zakir Ullah**, "Thermal-Isomerization Dynamics in Azobenzene Hydrogels under Irradiation" Functional Molecular Photoswitches for Energy Storage and Beyond, Barcelona Spain **2024**.

Skills:

Molecular dynamics and Quantum Mechanics packages: Maestro-Desmond, SYBYL, Material Studio, Jaguar, Gaussian, Qchem, Quantum ATK, ADF, MultiWfn.
Synthesis and Analysis: NMR, IR, Mass, UV-Vis, Fluorescence, CD, Crystallography, BET, TGA, Optical Microscope, DSC.
General Computer Skills: Basic Python, Basic Linux.

Certificates:

1. Crash Course on Python: https://www.coursera.org/account/accomplishments/certificate/YXXATEPRJF6T
2. Homogeneous Catalysis and Reactivity: https://courses.schrodinger.com/certificates/xrpklndwjy
3. Organic Electronics: https://courses.schrodinger.com/certificates/gztjkpljfe
4. Pharmaceutical Formulations: https://courses.schrodinger.com/certificates/hys3bgit9q
5. Surface Chemistry: https://courses.schrodinger.com/certificates/wviqwhswrl

Awards:

1. Prime minister (PaK) laptop scheme for highly talented students (M. Phil) (**2014**)
2. KAIST Special student scholarship (For my PhD.) (**2016-21**)
3. Seoul of the group award from KAIST Chemistry (**2018**)
4. Research program for excellence at Incheon National University, South Korea (**2021-22**)

5. Juan de la Cierva fellowship (**2023**)
6. Seal of excellence from Marie Curie fellowship (**2023**)

References:

1. **Prof**. David B. Amabilino
   - Professor of Smart Molecular, Inorganic and Hybrid Materials (ICMAB-CSIC, Spain)
   - Webpage: https://icmab.es/amabilino-david-brian
   - Email: amabilino@icmab.es

2. **Prof**. Hyun You Kim
   - Professor of Materials Science and Engineering, Chungnam National University (C.N.U. Republic of Korea)
   - Webpage: www.cnucmsl.com
   - Email: kimhy@cnu.ac.kr

3. **Prof**. Mihyun Kim
   - Associate Professor of Pharmacy
   - College of Pharmacy, Gachon University, Republic of Korea.
   - Webpage: https://sites.google.com/site/gacheondrlab/home
   - Email: kmh0515@gachon.ac.kr

4. **Prof**. David G. Churchill
   - Professor of Bioorganic and Molecular Neurodegenerative Research (KAIST, Republic of Korea)
   - Webpage: http://churchill.kaist.ac.kr
   - Email: dchurchill@kaist.ac.kr

5. **Prof**. Khurshid Ayub
   - Associate Professor of Physical Organic Chemistry
   - COMSATS University, Abbottabbad Campus, KPK, Pakistan, 22060
   - Webpage: https://ctcrl.com
   - Email: khurshid@cuiatd.edu.pk