

Career Highlights

Dr. Rasheed Ahmad Khera

Honors/Awards

- Ph.D. from Germany was evaluated as *Magna cum laude*.
- M.Phil. from QAU-Islamabad, Pakistan with distinction.
- M.Sc. from BZU-Multan, Pakistan with distinction.
- Merit scholarship throughout academic period from primary school to Ph.D.
- Awarded one of the most prestigious German scholarships (DAAD) for Ph.D.
- Research Productivity Award in **2013** from Pakistan Council for Science and Technology.
- Research Productivity Award in **2012** from Pakistan Council for Science and Technology.
- Research Productivity Award in **2011** from Pakistan Council for Science and Technology.

As Teacher

- 13 Years of teaching experience
- Offered 3 different Ph.D. courses.
- Offered 4 different M.Phil. courses.
- Offered 4 different M.Sc. courses.
- Offered 2 different F.Sc. courses.
- Offered 10 different BS. courses.
- Designed entirely new Advisor for BS./M.Phil/Ph.D. courses.

As Researcher

- Research guidance of 20 M.Sc. research reports.
- **Supervision of 4 Ph.D. theses.**
- **Supervised 120 M.Phil. theses.**
- Completed 3 research projects as Principal Investigator by receiving funding from national agency (HEC).
- Shared research findings with the chemist's community by making **20 oral presentations** (plenary, invited, lectures) at including 10 different workshops/expos, where participated as Resource person.
- Published **129 research papers** in ISI journals of impact factor in Q1, Q2, Q3 and Q4 category journals.
- Established strong research collaboration at national and international level.

Curriculum Vitae

What you are is God’s gift to you, what you make yourself is your gift to God.

Personal

Name	Dr. Rasheed Ahmad Khera
Father’s Name	Hafiz Elahi Bakhsh Khera (Late)
Date & Place of Birth	15-04-1980, Muzaffargarh.
Nationality	Pakistani
CNIC	32304-5067825-1
Passport Number	AM-4128252
Occupation	Teaching, Research, Planning science & technology
Mailing Address	Department of Chemistry, University of Agriculture, Faisalabad, Pakistan. Phone +923016645145 E-mail: rasheedahmadkhera@yahoo.com
Permanent Address	Basti Kotla Sadat P/O Langer Sarey, Tehsil and District Muzaffargarh, Punjab, Pakistan

Academic Qualifications

Examination	Period	Board/University	Division/Grade
Ph.D.	Nov. 2010	University of Rostock, Germany	Magna cum laude (very good)
M.Phil.	Dec. 2006	Quaid-i-Azam University, Islamabad, Pakistan	1 st
M.Sc.	Apr. 2004	Bahauddin Zakariya University Multan, Pakistan	1 st
B.Sc.	Aug. 2001	Bahauddin Zakariya University Multan, Pakistan	2 nd
F.Sc.	Aug. 1999	Multan Board	2 nd
SSC	Jun. 1996	Multan Board	1 st

Titles of Theses

Ph.D.	Synthesis of Functionalized Triarylmethanes and Pyranones Based on Cyclization Reactions of Free and Masked Dianions and Regioselective Palladium(0)-Catalyzed Reactions of Functionalized Sulfones, Benzophenones, Pyrazoles, Indenones, and Furans
M.Phil.	Combinatorial synthesis and biological screening of small drug-like molecules.
M.Sc.	Preparation and characterization of some isoniazid incorporated schiff bases and their transition metal complexes

Publications

1. Ahmad Raza, Muhammad Ans, Rasheed Ahmad Khera, R. Bousbih, Muhammad Waqas, Mohammed Aljohani, Mohammed A. Amin, Ali S. Alshomrany, Saba Zahid, Mohamed Shaban, *Journal of Molecular Modeling*, **2024**, 30, 190, Designing efficient materials for high-performance of non-fullerene organic solar cells through side-chain engineering on DBT-4F derivatives by non-fused-ring electron acceptors.
2. Sajjad Ali, Muhammad Salim Akhter, Muhammad Waqas, Hira Zubair, Haq Nawaz Bhatti, Ahmed Mahal, Ahmed M. Shawky, Anas Alkhouri, Rasheed Ahmad Khera, *Journal of Molecular Graphics and Modelling*, **2024**, 127, 108699, End-capped engineering of Quinoxaline core-based non-fullerene acceptor materials with improved power conversion efficiency.
3. Hira Zubair, Muhamed Salim Akhter, Muhammad Waqas, Mariam Ishtiaq, Ijaz Ahmed Bhatti, Javed Iqbal, Ahmed M. Skawky, **Rasheed Ahmad Khera***, *Journal of Molecular Graphics and Modelling*, **2024**, 126, 108664, A computational insight into enhancement of photovoltaic properties of non-fullerene acceptors by end-group modulations in the structural framework of INPIC molecule.
4. Faseh ur Rehman, Muhammad Waqas, Muhammad Imran, Mahmoud A. A. Ibrahim, Javed Iqbal, **Rasheed Ahmad Khera***, N. M. A. Hadia, Sameerah I. Al-Saeedi, and Mohamed Shaban, *ACS Omega* **2023**, 8, 43792–43812, Approach toward Low Energy Loss in Symmetrical Nonfullerene Acceptor Molecules Inspired by Insertion of Different π -Spacers for Developing Efficient Organic Solar Cells.
5. Jaweria Rukhsar, Muhammad Waqas, Muhamed Salim Akhter, Mohamed Shaban, Sameerah I. Al-Saeedi, Muhammad Shabir Mahr, Tamer H. A. Hasanin, Mahmoud A. A. Ibrahim, Naifa S. Alatawi, **Rasheed Ahmad Khera***, *The Journal of Physical Organic Chemistry*, **2023**, 4587, A DFT approach toward designing selenophene-based unfused small molecule acceptors by end-capped modification for improving the photovoltaic performance of organic solar cells.
6. Maham Majeed, Muhammad Waqas, Zouhaier Aloui, Manel Essid, Mahmoud A. A. Ibrahim, **Rasheed Ahmad Khera***, Mohamed Shaban, and Muhammad Ans, *ACS Omega*, **2023**, 8, 48, 45384-45404, Exploring the Electronic, Optical, and Charge Transfer Properties of A-D-A-Type IDTV-ThIC-Based Molecules to Enhance Photovoltaic Performance of Organic Solar Cells.
7. Faseh ur Rehman, Muhammad Waqas, Muhammad Imran, Mahmoud A. A. Ibrahim, Javed Iqbal, **Rasheed Ahmad Khera***, N. M. A. Hadia, Sameerah I. Al-Saeedi, and Mohamed Shaban, *ACS Omega*, **2023**, 8, 46, 43792–43812, Approach toward Low Energy Loss in Symmetrical Nonfullerene Acceptor Molecules Inspired by Insertion of Different π -Spacers for Developing Efficient Organic Solar Cells.
8. Ayesha Idrees, Ateeq-ur-Rehman, Muhammad Waqas, Mohamed Shaban, Sameerah I. Al-Saeedi, Naifa S. Alatawi, Mahmoud A. A. Ibrahim, Tamer H. A. Hasanin, N.M.A. Hadia, and **Rasheed Ahmad Khera***, *Journal of Computational Biophysics and Chemistry*, **2023**,

- 22, 08, 1041-1066, Strategies Toward End-group Engineering of Chrysene Core-based Non-fullerene Acceptors for High Performance Organic Solar Cells: A DFT Study.
9. Raheela Sharafat, Arslan Basharat, Ume Salma, Javed Iqbal, **Rasheed Ahmad Khera**, Ibrahim A. Shaaban, Mohammed A. Assiri, Lamia Abu El Maati, *Journal of Physics and Chemistry of Solids*, **2023**, 186, 111798, Investigating the impact of end-capped acceptor alterations to dimethyl fluorene-based hole transporting material for perovskite solar cells.
 10. Raheela Sharafat, Rao Aqil Shehzad, Muneerah Alomar, Rabia Shakeel, Tayyba Khalid, Javed Iqbal, Rasheed Ahmad Khera, *Optik*, **2023**, 295, 171537, End-capped engineering of carbazole based dopant free hole transporting material with improved power conversion efficiency.
 11. Faseh Ur Rehman, Shanza Hameed, **Rasheed Ahmad Khera***, Mohamed Shaban, Manel Essid, Zouhaier Aloui, Sameerah I. Al-Saeedi, Mahmoud A. A. Ibrahim, and Muhammad Waqas, *ACS Omega*, **2023**, 8, 45, 42492–42510, High-Efficiency and Low-Energy-Loss Organic Solar Cells Enabled by Tuning the End Group Modification of the Terthiophene-Based Acceptor Molecules to Enhance Photovoltaic Properties.
 12. Ramsha Ali, Sidra Nadeem, **Rasheed Ahmad Khera**, Abeer A. AlObaid, Ismail Warad, Mahmoud A. A. Ibrahim, and Muhammad Waqas, *Journal of Computational Biophysics and Chemistry*, **2023**, 22, 08, 1013-1040, An Approach Towards Low Energy Loss by End-capped Modification of A2-D–A1–D–A2-type Molecules for Tuning the Photovoltaic Properties of Organic Solar Cells.
 13. Amna Zahoor, Sonia Sadiq, **Rasheed Ahmad Khera**, Manel Essid, Zouhaier Aloui, Naifa S. Alatawi, Mahmoud A.A. Ibrahim, Tamer H.A. Hasanin, Muhammad Waqas, *Journal of Molecular Graphics and Modelling*, **2023**, 108613, A DFT study for improving the photovoltaic performance of organic solar cells by designing symmetric non-fullerene acceptors by quantum chemical modification on pre-existed LC81 molecule.
 14. Hira Zubair, Rana Farhat Mahmood, Muhammad Waqas, Mariam Ishtiaq, Javed Iqbal, Mahmoud A. A. Ibrahim, Shaban R. M. Sayed, Sadia Noor and **Rasheed Ahmad Khera**, *RSC Advances*, **2023**, 13, 26050-26068, Effect of tailoring π -linkers with extended conjugation on the SJ-IC molecule for achieving high VOC and improved charge mobility towards enhanced photovoltaic applications.
 15. Sabiha Khanam, Sahar Javaid Akram, **Rasheed Ahmad Khera***, Sadia Tul Zohra, Ahmed M. Shawky, Naifa S. Alatawi, Mahmoud A.A. Ibrahim, Ehsan Ullah Rashid, *Journal of Molecular Graphics and Modelling*, **2023**, 125, 108580 “Exploration of charge transfer analysis and photovoltaics properties of A-D-A type non-fullerene phenazine based molecules to enhance the organic solar cell properties”.
 16. Shanza Hameed, Muhammad Waqas, Saba Zahid, Shehla Gul, Ahmed M. Shawky, Naifa S. Alatawi, Rao Aqil Shehzad, Ijaz Ahmed Bhatti, Khurshid Ayub, Javed Iqbal, **Rasheed Ahmad Khera***, *Journal of Molecular Graphics and Modelling*, **2023**, 123, 108505, “Quantum Chemical Approach of Hexaammine (NH₃)₆ complexant with alkali and alkaline earth metals for their potential use as NLO materials”.
 17. Mehvish Perveen, Lubna Noreen, Muhammad Waqas, Rana Farhat Mehmood, Javed Iqbal, Sidra Manzoor, Sidra Nazir, Ahmed M. Shawky, **Rasheed Ahmad Khera***, *Journal of*

Molecular Graphics and Modelling, **2023**, *124*, 108537, “A DFT approach for finding therapeutic potential of graphyne as a nanocarrier in the doxorubicin drug delivery to treat cancer”.

18. Muhammad Hamza Maqsood, **Rasheed Ahmad Khera***, Rana Farhat Mehmood, Sahar Javaid Akram, Nabil Al-Zaqri, Mahmoud A.A. Ibrahim, Sadia Noor, Muhammad Waqas, *Journal of Molecular Graphics and Modelling*, **2023**, *124*, 108550, “End-cap modeling on the thienyl-substituted benzodithiophene trimer-based donor molecule for achieving higher photovoltaic performance”.
19. Maham Majeed, Muhammad Waqas, Rana Farhat Mehmood, Naifa S. Alatawi, Manel Essid, **Rasheed Ahmad Khera***, *Journal of Physics and Chemistry of Solids*, **2023**, *181*, 111495, Modified optoelectronic parameters by end-group engineering of A-D-A type non-fullerene-based small symmetric acceptors constituting IBDT core for high-performance photovoltaics.
20. Mariam Ishtiaq, Muhammad Waqas, Hira Zubair, Rana Farhat Mehmood, Nabil Al-Zaqri, **Rasheed Ahmad Khera***, Mahmoud A.A. Ibrahim, Javed Iqbal, *Journal of Molecular Liquids*, **2023**, *386*, 122473. “Theoretical designing of symmetrical non-fullerene acceptor molecules by end-capped modification for promising photovoltaic properties of organic solar cells”.
21. Ahmad Raza, Rana Farhat Mehmood, Ehsan Ullah Rashid, Samia Nasr, I.S. Yahia, Javed Iqbal, Naifa S. Alatawi, **Rasheed Ahmad Khera***, *Journal of Molecular Graphics and Modelling*, **2023**, *124*, 108563, “Amplifying the photovoltaic properties of phenylene dithiophene core based non-fused ring by engineering the terminal acceptors modification to enhance the efficiency of organic solar cells”.
22. Amna Zahoor, N. M. A. Hadia, Sahar Javaid Akram, Rana Farhat Mehmood, Sonia Sadiq, Ahmed M. Shawky, Naifa S. Alatawi Asma Ahmed, Javed Iqbal, **Rasheed Ahmad Khera***, *RSC Advances*, **2023**, *13*, 6530, Alteration of the central core of a DF-PCIC chromophore to boost the photovoltaic applications of non-fullerene acceptor based organic solar cells.
23. Mehvish Perveen, N.M.A. Hadia, Asima Noreen, Rana Farhat Mehmood, Samia nasr, I.S. Yahia, **Rasheed Ahmad Khera***, Javed Iqbal, *Journal of Molecular Graphics and Modelling*, **2023**, *121*, 108452, Controlled supramolecular interactions for targeted release of Amiodarone drug through Graphyne to treat cardiovascular diseases: An in silico study
24. Sahar Javaid Akram, N. M. A. Hadia, Ahmed M. Shawky, Javed Iqbal, Muhammad Imran Khan, Naifa S. Alatawi, Mahmoud A. A. Ibrahim, Muhammad Ans, and **Rasheed Ahmad Khera***, *ACS Omega*, **2023**, *8*, *12*, 11100-11117, Designing of Thiophene [3, 2-b] Pyrrole Ring-Based NFAs for High-Performance Electron Transport Materials: A DFT Study.
25. Muhammad Imran Khan, N.M.A. Hadia, Javed Iqbal, Sahar Javaid Akram, M. M. Hessien, Ahmed M. Shawky, Zouhaier Aloui, Naifa S. Alatawi, **Rasheed Ahmad Khera***, *Journal of Solid State Chemistry*, **2023**, *317*, 123714, Novel A- π -D- π -A-type non-fullerene acceptors for solution-processed organic photovoltaic cells: A DFT study
26. Muhammad Waqas, N. M. A. Hadia, Ahmed M. Shawky, Rana Farhat Mahmood, Manel Essid, Zouhaier Aloui, Naifa S. Alatawi, Javed Iqbal, **Rasheed Ahmad Khera***, *RSC Advances*, **2023**, *13*, 7535, Theoretical framework for achieving high Voc in non-fused

non-fullerene terthiophene-based endcapped modified derivatives for potential applications in organic photovoltaics.

27. Mafia Rani, N. M. A. Hadia, Ahmed M. Shawky, Rana Farhat Mehmood, Shanza Hameed, Saba Zahid, Javed Iqbal, Naifa S. Alatawi, Asma Ahmed, **Rasheed Ahmad Khera***, RSC Advances, **2023**, 13, 1640, Novel A-p-D-p-A type non-fullerene acceptors of dithienyl diketopyrrolopyrrole derivatives to enhance organic photovoltaic applications: a DFT study.
28. Muhammad Imran Khan, N.M.A. Hadia, Ahmed M. Shawky, M. M. Hessien, Manel Essid, Sahar Javaid Akram, Javed Iqbal, Naifa S. Alatawi, Gaber A. M. Mersal, **Rasheed Ahmad Khera***, Journal of Physics and Chemistry of Solids, **2023**, 174, 111140, Quantum mechanical modeling of fused rings-based small-donor molecules with enhanced optoelectronic attributes for high performance organic photovoltaic cells.
29. Ehsan Ullah Rashid , Nabil Al-Zaqri, Ahmed Boshala, Ismail Warad, Javed Iqbal, Muhammad Ans, Muhammad Rizwan, Mahmoud A.A. Ibrahim, **Rasheed Ahmad Khera***, *Computational and Theoretical Chemistry*, **2023**, 1220 114001, End-group engineering of non-fused benzothiadiazol derivatives with thiophene rings based small donor molecules for tuning the photovoltaic properties via DFT approach
30. Saima Rani, Nabil Al-Zaqri, Javed Iqbal, Sahar Javaid Akram, Ahmed Boshala, Rana Farhat Mehmood, Muhammad Umar Saeed, Ehsan Ullah Rashid, **Rasheed Ahmad Khera***, RSC Advances, **2022**, 12, 29300, Designing dibenzosilole core based, A2- π -A1- π -D- π -A1- π -A2 type donor molecules for promising photovoltaic parameters in organic photovoltaic cells.
31. Muhammad Waqas, N.M.A. Hadia, M.M. Hessien, Javed Iqbal, Gaber A. M. Mersal, Shanza Hameed, Ahmed M. Shawky, Zouhaier Aloui, Mahmoud A. A. Ibrahim, **Rasheed Ahmad Khera***, Journal of Molecular Liquids, **2022**, 368, 120770, End-group modification of terminal acceptors on benzothiadiazolebased BT2F-IC4F molecule to establish efficient organic solar cells.
32. Muhammad Umar Saeed, N. M. A. Hadia, Javed Iqbal, M. M. Hessien, Ahmed M. Shawky, Muhammad Ans, Naifa S. Alatawi, **Rasheed Ahmad Khera***, Impact of end-group modifications and planarity on BDP-based non-fullerene acceptors for high-performance organic solar cells by using DFT approach.
33. Shanza Hameed, Shehla Gul, Muhammad Ans, Ijaz Ahmed Bhatti, Khurshid Ayub, Javed Iqbal, **Rasheed Ahmad Khera***, Journal of Molecular Modeling, **2022**, 28, 381, Designing neodymium-doped hexamine complexant as novel IR NLO material with extremely large non-linear optical behavior.
34. Ehsan Ullah Rashid, N. M. A. Hadia, Omaymah Alaysuy, Javed Iqbal, M. M. Hessien, Gaber A. M. Mersal, Rana Farhat Mehmood, Ahmed M. Shawky, Muhammad Imran Khan, **Rasheed Ahmad Khera***, RSC Advances, **2022**, 12, 28608-28622, Quantum chemical modification of indaceno dithiophene-based small acceptor molecules with enhanced photovoltaic aspects for highly efficient organic solar cells.
35. Muhammad Umar Saeed, Javed Iqbal, Rana Farhat Mehmood, Muhammad Riaz, Sahar Javaid Akram, H. H. Smailly, Ahmed M. Shawky, Muhammad Raheel, Muhammad Imran

- Khan, Ehsan Ullah Rashd, **Rasheed Ahmad Khera***, *Journal of Physics and Chemistry of Solids*, **2022**, *170*, 110906, Structural modification on Dimethoxythienothiophene based non-fullerene acceptor molecule for construction of high-performance organic chromophores by employing DFT approach.
36. Abid Hussain, N. M. A. Hadia, M. M. Hessien, **Rasheed Ahmad Khera****, Saba Zahid, Rao Aqil Shehzad, Ali Raza Ayub Khurshid Ayub, Javed Iqbal, *Journal of Molecular Structure*, **2022**, *1270*, 133910, DFT study of super-halogen (Al7) doped carbon nitride (C2N) and its nonlinear optical properties.
 37. Muhammad Waqas, Javed Iqbal, Rana Farhat Mehmood, Sahar Javaid Akram, Ahmed M. Shawky, Muhammad Raheel, Ehsan Ullah Rashid, **Rasheed Ahmad Khera****, *Journal of Molecular Graphics and Modelling*, **2022**, *116*, 108255. Impact of end-capped modification of MO-IDT based non-fullerene small molecule acceptors to improve the photovoltaic properties of organic solar cells.
 38. Muhammad Waqas, N. M. A. Hadia, M. M. Hessien. Sahar Javaid Akram, Ahmed M. Shawky, Javed Iqbal, Mahmoud A. A. Ibrahim, **Rasheed Ahmad Khera****, *Computational and Theoretical Chemistry*, **2022**, 113904, Designing of symmetrical A-D-A type non-fullerene acceptors by side-chain engineering of an indacenodithienothiophene (IDTT) core-based molecule: A computational approach.
 39. Saliha Sabir, N. M. A. Hadia, Javed Iqbal, Rana Farhat Mehmood, Sahar Javaid Akram, Muhammad Imran Khan, Ahmed M. Shawky, Muhammad Raheel. H. H. Smailly, **Rasheed Ahmad Khera****, *Chemical Physics Letters*, **2022**, *806*, 140026. DFT molecular modeling of A2-D-A1-D-A2 type DF-PCIC based small molecules acceptors for organic photovoltaic cells.
 40. Zeeshana Bibi, Javed Iqbal, **Rasheed Ahmad Khera****, Muhammad Asgher, Spirothienoquinoline-based acceptor molecular systems for organic solar cell applications: DFT investigation, *Journal of Molecular Modeling*, **2022**, *28*, 244.
 41. Sahar Javaid Akram, N. M. A. Hadia, Javed Iqbal, Rana Farhat Mehmood, Saleem Iqbal, Ahmed M. Shawky, Areeba Asif, H. H. Smailly, Muhammad Raheel, **Rasheed Ahmad Khera****, *RSC Advances*, **2022**, *12*, 20792–20806, Impact of various heterocyclic p-linkers and their substitution position on the opto-electronic attributes of the A- π -D- π -A type IECIO-4F molecule: a comparative analysis
 42. Muhammad Usman Khan, Muhammad Khalid, **Rasheed Ahmad Khera****, Muhammad Nadeem Akhtar, Amna Abbas, Muhammad Fayyaz ur Rehman, Ataulpa Albert Carmo Braga, Mohammed Mujahid Alam, Muhammad Imran. Yao Wang, Changrui Lu., *Arabian Journal of Chemistry*, **2022**, *15*, 103673, Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A-[π]-D-[π]-D architecture.
 43. Iqra Zubair, **Rasheed Ahmad Khera****, Ayesha Naveed, Rao Aqil Shehzad, Javed Iqbal, *Materials Science in Semiconductor Processing*, **2022**, *148*, 106812, Designing the optoelectronic properties of BODIPY and their photovoltaic applications for high performance of organic solar cells by using computational approach.

44. Ayesha Naveed, Sahar Javaid Akram, Muhammad Ans, Javed Iqbal, Ifrah Batool, Rana Farhat Mehmood, **Rasheed Ahmad Khera****, *Journal of Molecular Modeling*, **2022**, 28, 218 Impact of end capped modification on BT-CIC molecule for high-performance photovoltaic attributes: A DFT approach.
45. Sahar Javaid Akram, Javed Iqbal, Muhammad Ans, Yaser A.El-Badry, Rana Farhat Mehmood, **Rasheed Ahmad Khera****, *Solar Energy*, **2022**, 237, 108-121, Designing of the indacenodithiophene core-based small molecules for optoelectronic applications: A DFT approach.
46. Mahnoor Qaisar, Shabbir Muhammad, Javed Iqbal, **Rasheed Ahmad Khera****, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, Muhammad Khalid and Fatima Hussain, *Journal of Computational Biophysics and Chemistry*, **2022**, 21, 139-153, Identification of Marine Fungi-Based Antiviral Agents as Potential Inhibitors of SARS-CoV-2 by Molecular Docking, ADMET and Molecular Dynamic Study.
47. Muhammad Usman Khan, Muhammad Khalid, Iqra Shafiq, **Rasheed Ahmad Khera****, Zahid Shafiqe, Rifat Jawaria, Muhammad Shafiq, Mohammed Mujahid Alam, Ataulpa Albert Carmo Braga, Muhammad Imran, Fariha Kanwal, Zhengjie Xu, Changrui Lu. *Journal of Saudi Chemical Society*, **2021**, 25, 101339, Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine-based D- π -A organic compounds and their derivatives.
48. Urwah Azeem, **Rasheed Ahmad Khera****, Ayesha Naveed, Muhammad Imran, Mohammed A. Assiri, Muhammad Khalid, Javed Iqbal, *ACS Omega* **2021**, 43, 28923-28935, Tuning of a A-A-D-A-A-Type Small Molecule with Benzodithiophene as a Central Core with Efficient Photovoltaic Properties for Organic Solar Cells.
49. Tehreem Asif, **Rasheed Ahmad Khera****, Ayesha Naveed, Maham Salim, Javed Iqbal, *Optik*, 247, **2021**, 167892, Tuning the optoelectronic properties of naphthodithiophene (NDT) for designing of A-D-A type photovoltaic materials.
50. Maham Salim, Mahira Rafiq, Yaser A. El-Badry, **Rasheed Ahmad Khera****, Muhammad Khalid, Javed Iqbal, *Journal of Molecular Modeling*, **2021**, 27, 316, Tuning the optoelectronic properties of ZOPTAN core-based derivatives by varying acceptors to increase efficiency of organic solar cell.
51. Mahira Rafiq, **Rasheed Ahmad Khera****, Maham Salim, Muhammad Khalid, Khurshid Ayub, Javed Iqbal, *Chemical Physics Letters*, **2021**, 782, 139018, Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications.
52. Aamer Saeed, Shafi Ullah Khan, Maria Saeed, Ghulam Shabir, Abbas Hasan, **Rasheed Ahmad Khera***, Hesham El-Seedi, Sobia Ahsan Halim, Ajmal Khan, Ahmed Al-Harrasi, Jamshed Iqbal, *Drug Dev Res.* **2022**;83:745–754, Synthesis of novel hybrid pharmacophore of N -((4-sulfamoylphenyl)carbamothioyl)alkanamides as potent carbonic anhydrase-II and 15-lipoxygenase inhibitors
53. Khadija Asif, Mehvish Perveen, **Rasheed Ahmad Khera***, Sidra Nazir, Ali Raza Ayub, Tehreem Asif, Muhammad Shabbir, Javed Iqbal, *Computational and Theoretical*

Chemistry, **2021**, 1206, 113459, Computational and theoretical study of graphitic carbon nitride (g-C₃N₄) as a drug delivery carrier for Isoniazid drug to treat cancer.

54. Anjum Ihsan*, **Rasheed Ahmad Khera***, Javed Iqbal and Muhammad Asghar, Z. Phys. Chem. **2022**; 236(4): 561–581, Binding interaction of benzamide derivatives as inhibitors of DNA gyrase and Sec14p using Molegro Virtual Docker based on binding free energy,
55. Maham Salim, Mahira Rafiq, **Rasheed Ahmad Khera****, Maira Arshad, Javed Iqbal, Solar Energy, **2022**, 233, 31-45, Amplifying the photovoltaic properties of azaBODIPY core based small molecules by terminal acceptors modification for high performance organic solar cells: A DFT approach
56. Muhammad Umar Saeed, Javed Iqbal, Rana Farhat Mehmood, Sahar Javaid Akram, Yaser A.El-Badry, Sadia Noor, **Rasheed Ahmad Khera***, Surfaces and Interfaces, **2022**, 30, 101875, End-capped modification of Y-Shaped dithienothiophen[3,2-b]-pyrrolobenzothiadiazole (TPBT) based non-fullerene acceptors for high performance organic solar cells by using DFT approach.
57. Ehsan Ullah Rashid, Javed Iqbal, Rana Farhat Mehmood, Yaser A.El-Badry, Sahar Javaid Akram, **Rasheed Ahmad Khera****, *Computational and Theoretical Chemistry*, **2022**, 1211, 113669, Depicting the role of end-capped acceptors to amplify the photovoltaic properties of benzothiadiazole core-based molecules for high-performance organic solar cell applications.
58. Iqra Zubair, **Rasheed Ahmad Khera****, Sahar Javaid Akram, Yaser A.El-Badry, Muhammad Umar Saeed, Javed Iqbal, Chemical Physics Letters, **2022**, 793, 139459, Tuning the optoelectronic properties of indacenodithiophene based derivatives for efficient photovoltaic applications: A DFT approach.
59. Muhammad Rais Aslam, **Rasheed Ahmad Khera****, Yaser A. El-Badry, Mahira Rafiq, Ayesha Naveed, Muhammad Tariq Shehzad, Javed Iqbal Journal of Molecular Graphics and Modelling, **2022**, 112, 108146, Tuning of diphenylamine subphthalocyanine based small molecules with efficient photovoltaic parameters for organic solar cells,
60. Aneesa Shahzadi, Javed Iqbal, Sahar Javaid Akram, Alvina Rasool, Yaser A. El-Badry, **Rasheed Ahmad Khera****, Journal of Molecular Modeling, **2022**, 28: 132, Symmetrical end-capped molecular engineering of star-shaped triphenylamine-based derivatives having remarkable photovoltaic properties for efficient organic solar cells.
61. Mafiah Rani, Javed Iqbal, Rana Farhat Mehmood, Ehsan Ullah Rashid, Misbah, Saima Rani, Muhammad Raheel, **Rasheed Ahmad Khera****, *Computational and Theoretical Chemistry*, **2022**, 1213, 113747, Strategies toward the end-group modifications of indacenodithiophene based non-fullerene small molecule acceptor to improve the efficiency of organic solar cells; a DFT study.
62. Talha Ishfaq, **Rasheed Ahmad Khera****, Saba Zahid, Umer Yaqoob, Rao Aqil Shehzad, Khurshid Ayub, Javed Iqbal, *Computational and Theoretical Chemistry*, Enhancement in non-linear optical properties of carbon nitride (C₂N) by doping superalkali (Li₃O): *Computational and Theoretical Chemistry*, **2022**, 1211, 113654, A DFT study.
63. Ayesha Tajammal, Muhammad Ans, Rana Farhat Mehmood, Javed Iqbal, Sahar Javaid Akram, Arifa Murtaza, **Rasheed Ahmad Khera****, *Computational and Theoretical*

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