Dr. Muhammad Adnan Asghar

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Profile Summary

Dr Muhammad Adnan Asghar is an **Associate Professor** (Tenured) of Chemistry, Department of Chemistry, Division of Science and Technology, University of Education, College Road, Lahore-Pakistan. He received his M.Sc. (2010) from University of the Punjab, Lahore and M.Phil. (2013) from Bahauddin Zakariya University, Multan and PhD (2016) from University of the Chinese Academy of Sciences, Beijing, China in Chemistry. He has more than 10 years of professional experience not limited to teaching and research but also in administration at university/college level. He has published **71 international research articles** as author/co-author/corresponding author in international peer reviewed journals, resulted in **2200+ citations**, **Impact factor = 325.8**, h-index = 23 and i10-index = 42. He has reviewed many research articles for internationally reputed journals and handled 02 journals as an associate editor.

Google Scholar.
https://scholar.google.com.pk/citations?hl=en&user=ggxr614AAAAJ&view_op=list_works&sortby=pubdate

Education

- **PhD (Inorganic Chemistry). 2016**

University of Chinese Academy of Sciences, China

(Fujian Institute of Research on the Structure of Matter, Fuzhou)

- **M. Phil. (Chemistry). 2013**

Bahauddin Zakariya University, Pakistan

(Division of Inorganic Chemistry, Institute of Chemical Sciences)

Major: Inorganic Chemistry

Professional, Teaching & Research Experience

- **Associate Professor (Tenured):** Department of Chemistry, Division of Science and Technology, University of Education, Lahore: November 14, 2023 to date
- **Assistant Professor (TTS):** Department of Chemistry, Division of Science and Technology, University of Education, Lahore: January 08, 2018 to November 13, 2023
- **Assistant Professor (IPFP):** Department of Chemistry, Division of Science and

Technology, University of Education, Lahore: February 01, 2017 to January 07, 2018.

Research Projects

Chemistry Courses Taught so far

Bachelor/Master Level (16 Years Education)

Fundamentals of Inorganic Chemistry (Theory and Lab) - (CHEM- 1111)
Fundamentals of Organic Chemistry (Theory and Lab) - (CHEM- 2061)
Industrial Chemistry (Theory and Lab) - (CHEM- 2081)
Chemistry of Transition Elements (Theory and Lab) - (CHEM-3111)
Inorganic Material Chemistry (Theory and Lab) - (CHEM-3115)
Inorganic Chemistry (Paper-I), (Theory and Lab) (CHEM- 4051)
Inorganic Reaction Mechanism (Theory) - (CHEM-4111)
Inorganic Spectroscopy (Theory) - (CHEM- 4115)
Organometallics (Theory) - (CHEM-4118)
Inorganic Chemistry (Paper-V), (Theory) - (CHEM-4056)
Symmetry and Magnetochemistry (Theory) - (CHEM-4120)

Master of Philosophy Level (18 Years Education)

Thermal Analysis – (CHEM 5137)
Advanced Inorganic Material Chemistry – (CHEM-5129)
Advanced Coordination Chemistry – (CHEM-5130)
Chemistry of Atmosphere - (CHEM-5149)

Ph.D. Level

Industrial Inorganic Pigments (Theory) for PhD Chemistry-IInd Semester (CHEM-7116)

M. Phil. Supervision (18-Years Education)

1. Green synthesis of Ni and Mn codoped ZnO nanoparticles and their composites with activated carbon for photocatalytic degradation of methylene blue. Tahira Iqbal (2025)
2. Development of biodegradable hydrogel-film derived from chitosan-curcumin containing black seed extract-ZnO Nps for packaging. Sehar Aftab (2025)
3. Effect of ($CaSO_4$-MgO-Modified SiO2) Filler Modified Epoxy Resin on Mechanical properties of Carbon Fiber Laminates. Arslan Umer (2024)
4. Synthesis of Iron based Metal Organic Frameworks for the Slow Release of Nitrogen based Fertilizers in Plants. Muhammad Tayyab Fida (2024)
5. Antibacterial and Antioxidant Applications of Ciprofloxacin and Linezolid Loaded Nitrophenyl furfural chitosan Based Hydrogels. Muhammad Nadir (2024)
6. Potential Human Health Risk Assessment Via consumption of Rice Planted in Toxic Metals Contaminated Soil. Muhammad Bilal (2023)
7. Photocatalytic Degradation of Methylene Orange using Co-doped ZnO@Ag-Co Nanoparticles. Anum Shahzadi (2023)
8. Green Synthesis OF Iron Doped Nickel Oxide Nanoparticles from OKRA (Abelmoscus esculentus) Plant Extract. Muhammad Hassan (2023)
9. Photo-catalytic Degradation of Methylene blue using Al-Cu codoped ZnO Nanoparticles. Nouman Rafique (2023)
10. Hydrothermally Grown Al and Fe codoped ZnO Nanoparticles for Photodegradation of

different basic dyes. Rabbia Saleem (2023)

11. Synthesis and Characterization of Ag dopedTiO_2 Graphene Nanocomposites and their photocatalytic activity under visible light source. Aneela Rasheed (2022)
12. Seed Mediated growth of Anatase TiO_2 Nanoparticles for Photocatalytic Activities. Sara Anjum (2022).
13. Hydrothermal Synthesis of Nickel based Phase Transition Materials and Study of their Anisotropic Properties. Muhammad Faisal (2022).
14. Hydrothermal Synthesis of Cobalt Based Phase Transition Materials and Study of their Anisotropic Properties. Humaira Gurmani (2022).
15. Photocatalytic Characteristics of Bi and Pb Co-doped TiO_2 Nanoparticles under Visible light. Seerat Ul Urooj (2019).
16. Photocatalytic Characteristics of Sb and Pb Co-doped TiO_2 Nanoparticles under Visible light. Riffat Shabbir (2019).
17. Synthesis, Characterization and Computational Modeling of Ni, Zn and Cd Based Phase Transition Materials. Abdul Majeed (2019).
18. Synthesis and Characterization of Inorganic-Organic Hybrid Phase Change Crystals. Sikander Hayat (2019).
19. Synthesis of Picric Acid Based Phase Transition Material. Muhammad Aslam (2018).

Academic Professional Activities

- Paper Setter, BS/MSc-Chemistry, University of Education, Lahore-Pakistan
- Member Research Proposal Review Committee, Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan
- Member University Sports Committee (Football), Sports Week, 28 March-01 April, 2022, University of Education, Lahore- Pakistan
- Member Admission Committee, Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan.
- Member Organizing Committee, 2nd International Conference on Trends and Research in Chemistry (TRIC-2023) held at University of Education, Lahore on 16-18 May 2023.
- Member Organizing Committee, 1st International Conference (online). Trends & Research in Chemistry (TRIC 2022), Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan: Jan. 18-19, 2022
- Organized One Day Webinar on "Analysis of Fermented Food by using NMR Technique" at University of Education Lahore, DG Khan Campus on 26-Feb-2021.
- Organized One Day Webinar on "Applications of Metal Organic Frameworks in Catalysis" at University of Education Lahore, DG Khan Campus on 11-Jan-2021.
- Organized One Day Webinar on "NMR Spectroscopy for the Analysis of Foods" at University of Education Lahore, DG Khan Campus on 30-Nov-2020.
- Organized One Day Seminar on "Material Chemistry" at University of Education Lahore, DG Khan Campus on 13-January-2020.
- Organized One Day Symposium on "Computational Chemistry" at University of Education Lahore, DG Khan Campus on 08-April-2019.
- Organized One Day Seminar on "Food Chemistry" at University of Education Lahore, DG Khan Campus on 10-Dec-2018.
- Organized One Day Seminar on "Recent Trends in Chemistry" at University of Education Lahore, DG Khan Campus on 10-May-2018.
- Program Team Member to Prepare Self-Assessment Report of MS-Chemistry for Year, 2021-2022, Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan
- External examiner for M.Phil thesis-University of the Punjab, Lahore

- External examiner for B.S. practical thesis-University of the Punjab, Lahore
- External examiner for M.Phil thesis- Bahauddin Zakariya University, Multan
- Research Assistant: Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences Fuzhou, P. R. China. April 2013 – August 2013
- Estate officer: University of Education Lahore, DG Khan Campus 15th Nov 2018-2021
- Focal Person-Financial Aid Office: University of Education Lahore, DG Khan Campus 12th Oct 2018- 2021
- In-charge : Main Library, University of Education (FSD Campus) 1ist Feb 2017- 07th Jan 2018
- In-charge : Computer Labs, University of Education (FSDCampus) 1ist Feb 2017- 07th Jan 2018

Editorship & Memberships

- Member Editorial Board of Frontiers in Materials (IF=3.2, ISSN 2296 8016)
- Worked as a "Guest Editor" at Crystals (IF =2.67, ISSN 2073 4352)
- Reviewer of RSC, ACS, Wiley, Elsevier and many other publishing groups.
- Member of Royal Society of Chemistry, London (Membership ID: 643941).
- Received Gold Medal in annual meeting of Zakariyan Chemist Organization (ZACHO), organized by Institute of Chemical Sciences, Bahauddin Zakariya University, Multan, Pakistan on 31ist March 2017.
- Awarded with Excellent International PhD Graduate of University of Chinese Academy of Sciences, Beijing in 2016.
- Secured meritorious University of Chinese Academy of Sciences (UCAS) Fellowship to pursue my PhD studies (2013-2016).
- One of my First Author article is honored as a "Hot Paper" in themed collection of Journal of Material Chemistry C, 2016.
- Got the Appreciation Certificate from French Ambassador on explaining the latest chemistry models in 2012

Workshops, Seminars & Conferences

1. Two day "Workshop on Project Formulation" organized by Pakistan Science Foundation (PSF) at FC University, Lahore on 24-25-May-2023.
2. Oral Presentation, Title: "Experimental and Theoretical Exploration of Non Linear Optical materials" 2nd International Conference, Trends & Research in Chemistry (TRIC 2023), Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan: Jan. 16-18 May, 2023
3. One day "Workshop on Electrochemical work-station Potentiostate" organized by University of Management Sciences (UMT) Lahore on 10-Feb-2022.
4. Oral Presentation, Title: Exploration of New Phase transition Martials (Jan. 19, 2022). 1st International Conference (online). Trends & Research in Chemistry (TRIC 2022), Department of Chemistry, Division of Science and Technology, University of Education, Lahore-Pakistan: Jan. 18-19, 2022
5. Capacity Building Workshop offered by Punjab Higher Education Commission and QAS

Foundation (29-Feb to 25-July 2020)

6. Higher Education Commission of Pakistan organized a workshop for the Evaluation Sheet and Pre ISAC, Shortlisting process of Ehsaas Undergraduate Scholarship Project on 15-01-2020 at Ghazi University DG Khan
7. Pak Institute for Peace Studies (PIPS) invites to participate in two-day dialogue on social harmony, at the Best Western Hotel, Lahore, on January 4th, 5th - 2019.
8. Oral Presentation. "Structural-Property relationship to determine the properties of phase transition materials" 6th International Conference on Education (Science Beyond Classroom) organized by University of Education, Lahore on 15-17, March 2018
9. Quality Enhancement Cell based SAR Program team members training workshop (14-16 May-2018).
10. 10th China-Japan Joint Symposium on Metal Cluster Compounds (CJSMCC-2015) held at FuZhou, China 23-26 October-2015.
11. Workshop on "Frontier of Green Technology" held at Institute of Processing Engineering, Chinese Academy of Sciences, Beijing, China (24-29 September-2013).
12. Presented a paper entitled "Hydrothermal synthesis and Characterization of novel 2-D and 3-D Carboxylate based Metal-Organic frameworks", M. Athar and Muhammad Adnan Asghar at University of Peshawar (2012),
13. Participation: 9th International and 21ist national Chemistry conference held at University of Karachi, Pakistan, on 14-16 March-2011
14. Participation: 10th international and 22nd National Chemistry Conference at University of Agriculture, Faisalabad, Pakistan, 21-22 November 2011.

Research Publications

Year 2025

1. **M. A. Asghar***, I. Shafiq, S. Jamal, K. A. Alrashidi, Ke Chen "Molecular engineering with benzothiophene based bracing units to improve the photovoltaic properties of the naphthalene core based chromophores" *Scientific Reports* 2025, 15, 26872. **[Impact Factor: 3.9]**
2. M. Khan, A. Tariq, I. Irshad, **M. A. Asghar***, T. Ahamad, Ke Chen "A DFT based insights for molecular designing of pyridine dipyrrolide core with benzodithiophene-based acceptors for organic solar cells" *Scientific Reports* 2025, 15, 25708. **[Impact Factor: 3.9]**
3. U. Aiman, M. Adeel, A. Hussain, A. Rauf, S. Hussain, A. Villingar, A. Amin, K. S. Munawar, S. M Alshehri, **M. A. Asghar*,** "Facile synthesis, SC-XRD, spectroscopic

characterization & key electronic properties of nicotinaldehyde based scaffolds" *Journal of Molecular Structure* 2025, 1321, 139744. **[Impact Factor: 4.0]**

4. **M. A. Asghar*,** A. Jabbar, S. Nadeem, I. Shafiq, N. Tahir, K. A. Alrashidi "Photovoltaic response promoted via intramolecular charge transfer in triphenylpyridine core with small acceptors: A DFT/TD-DFT study" *Materials Science in Semiconductor Processing* 2025, 186, 109086. **[Impact Factor: 4.2]**

Year 2024

5. I. Shafiq, R. Ahmed, I. Irshad, M. Haroon, N. Alhokbany, K. S. Munawar, **M. A. Asghar*,** "Theoretical study of star shaped benzotriindole based variant non-fullerene acceptors for efficient organic solar cells" *Optical and Quantum Electronics* 2024, 11, 56, 1800. **[Impact Factor: 3.3]**

6. S. Haq, **M. A. Asghar*,** I. Shafiq, M. Saeed, W. Anwer, M. Haroon, R. Alotaibi "Exploring the influence of fused heterocyclic donor moieties on optical nonlinearity of styrylthiophene based chromophores: A DFT study" *Computational and Theoretical Chemistry* 2024, 1240, 114788. **[Impact Factor: 3.0]**

7. S. Haq, U. Shoukat, I. Shafiq, **M. A. Asghar*,** M. Arshad, T. Ahamad, R. Baby, "Transmittal Effect Evaluation of Heterocyclic Rings on Nonlinear Optical Ambit of Benzotrithiophene-Based Push-Pull Driving Materials: a Theoretical Approach" *Polycyclic Aromatic Compounds* 2024, 8, 44, 5338-5361. **[Impact Factor: 2.4]**

8. I. Khan, M. Adeel, T. Ahamad, M. S. Khan, G. Schnakenburg, S. Ahmed, S. C. Ojha, **M. A. Asghar*,** "Synthesis, Characterization, and DFT Study of Mono-and Di-Arylated Pyridine Derivatives" *Polycyclic Aromatic Compounds* 2024, 7, 44, 4639-4662. **[Impact Factor: 2.4]**

9. M. Haroon, T. Akhtar, M. Khalid, H. Mehmood, **M. A. Asghar**, T. Ahamad, S. Ahmed, A. AC Braga "Synthesis, Spectroscopic and Quantum Chemical Studies of N-Pentylhydrazinylthiazole Derivatives" *Polycyclic Aromatic Compounds* 2024, 5, 44, 3178-3199. **[Impact Factor: 2.4]**

10. M. Khalid, S. Yasmeen, S. Ahmed, **M. A. Asghar**, M. Imran, A. A.C. Braga, S. Chandra Ojha "Improved the optical nonlinearity of carbazole based chromophores via molecular engineering: A DFT approach" *Arabian Journal of Chemistry*, 2024, 105753. **[Impact Factor: 6.221]**

11. M. Khalid, R. Maqsood, I. Shafiq, R. Baby, **M. A. Asghar*,** S. Ahmed, S. M Alshehri, A. AC Braga "Theoretical Approach towards Benzodithiophene-Based Chromophores with Extended Acceptors for Prediction of Efficient Nonlinear Optical Behaviour" *Arabian Journal for Science and Engineering*, 2024, 49, 339–359. **[Impact Factor: 2.87]**

12. M. Khalid, A. Mustafa, A. AC Braga, **M. A. Asghar**, N. Raza "Exploration of photovoltaic properties towards efficient organic solar cells for Thieno [3, 2-b] thiophene fused naphthalene core based acceptor derivatives" *Journal of Photochemistry and Photobiology A: Chemistry* 2024, 447, 115279. **[Impact Factor: 4.3]**

13. M. N. Tahir, M. Ashfaq, K. S. Munawar, A. U. Khan, **MA Asghar *** T. Ahamad, S. C. Ojha "Synthesis, Characterizations, Hirshfeld Surface Analysis, DFT, and NLO Study of a Schiff Base Derived from Trifluoromethyl Amine" *ACS Omega* 2024, 9 (2), 2325-2338. **[Impact Factor: 4.132]**

14. I. Shafiq, U. Shoukat, **MA Asghar**, M. Aslam, T. Ahamad, S. Ahmed, S. Bullo, S. C. Ojha "Structural Tailoring via End-capped Acceptors of Thiophene-based C-shaped Non-fullerene Compounds with A-π-A Backbone for the Exploration of Photovoltaic Response" *Journal of Saudi Chemical Society*, 2024, 101799. **[Impact Factor: 5.6]**

Year 2023

15. M. Khalid, R. Jawaria, S. A. Ditta, I. Shafiq, A. AC Braga, S. M Alshehri, **MA Asghar *** "Synthesis, characterization and exploration of optical non-linearity of secondary ketamine derivatives via DFT study" *Optical and Quantum Electronics* 2023, 55 (13), 1121. **[Impact Factor: 2.8]**

16. M. Khalid, I. Shafiq, **MA Asghar *,** A. A. C. Braga, S. M Alshehri, M. Haroon, M. L. Sanyang "Promising impact of push–pull configuration into designed octacyclic naphthalene-based organic scaffolds for nonlinear optical amplitudes: a quantum chemical approach" *Scientific Reports* 2023, 13 (1), 20104. **[Impact Factor: 4.996]**

17. I. Shafiq, R. Zahid, K. Mahmood, **MA Asghar *,** T. Ahamad, S. Ahmed, S. C. Ojha "Introducing the various electron withdrawing functions in trigging the optical nonlinearity of benzodithiophene based chromophores: A quantum chemical approach" *Journal of Saudi Chemical Society* 2023, 27 (6), 101767. **[Impact Factor: 5.6]**

18. M. Khalid, A. Mustafa, S. Ahmed, **M. A. Asghar**, T. Ahamad, A. AC Braga, S. C. Ojha "Photovoltaic response promoted via intramolecular charge transfer in pyrazoline-based small molecular acceptors: Efficient organic solar cells" *Arabian Journal of Chemistry* 2023, 16 (11), 105271. **[Impact Factor: 6.221]**

19. I Shafiq, M Khalid, N Raza, AAC Braga, M Khairy, **MA Asghar *** "Exploring promising photovoltaic properties of dithiophene-based non-fullerene chromophores for efficient organic solar cells: A DFT approach" *Synthetic Metals*, 2023, 299, 117455. **[Impact Factor: 4.0]**

20. I. Shafiq, A. Mustafa, R. Zahid, R. Baby, S. Ahmed, **M. A. Asghar*,** T. Ahamad, M. Alam, A. AC Braga, S. C. Ojha "Theoretical Perspective toward Designing of 5-Methylbenzo [1,2-b:3,4-b′:6,5-b″] trithiophene-Based Nonlinear Optical Compounds with Extended Acceptors" *ACS Omega* 2023, 8, 42, 39288–39302. **[Impact Factor: 4.132]**

21. I. Shafiq, M. Khalid, **M. A. Asghar**, R. Baby, A. AC Braga, S. M Alshehri, S. Ahmed "Influence of azacycle donor moieties on the photovoltaic properties of benzo[c][1,2,5]thiadiazole based organic systems: a DFT study" *Scientific Reports*, 2023, 13, 14630. **[Impact Factor: 4.996]**

22. S. Ahmed, I. Irshad, S. Nazir, S. Naz, **M. A. Asghar**, S. M Alshehri, S. Bullo, M. L. Sanyang "Designing of banana shaped chromophores via molecular engineering of terminal groups to probe photovoltaic behavior of organic solar cell materials" *Scientific Reports*, 2023, 13, 15064. **[Impact Factor: 4.996]**

23. I. Shafiq, U. H. Ishaque, M. Khalid, A. A. C. Braga, **M. A. Asghar**, S. M. Alshehri, S. Ahmed f, S. C. Ojha "A theoretical approach for exploration of non-linear optical amplification of fused azacycle donor based thiophene polymer functionalized chromophores" *Journal of Saudi Chemical Society*, 2023, 27, 5, 101707. **[Impact Factor: 5.6]**

24. M. A. U. Rehman, M. Adeel, S. M. Alshehri, U. Aiman, A. Villinger, S. Bullo, R. Baby, **M. A. Asghar**, A. E Kuznetsov, M. L. Sanyang "Novel Fluorinated Biphenyl Compounds Synthesized via Pd(0)-Catalyzed Reactions: Experimental and Computational Studies" *ACS Omega* 2023, 8, 32, 29414–29423. **[Impact Factor: 4.132]**

25. M. Haroon, T. Akhtar, Q. Shaikh, H. Mehmood, M. Khalid, **M. A. Asghar**, S M Alshehri, S. C. Ojha "Facile Synthesis and DFT Analysis of Novel Thiazole-Based Hydrazones: An Experimental and Theoretical Perspective" *ACS Omega* 2023, 8, 30, 27488–27499. **[Impact Factor: 4.132]**

26. H Mehmood, T Akhtar, M Haroon, M Khalid, AAC Braga, S Woodward, **M. A. Asghar** "Spectroscopic characterization and quantum-chemical analysis of hydrazinyl thiazol-4 (5H)-one functionalized materials to predict their key electronic and non-linear optical behavior" *Journal of Molecular Structure,* 2023, 1288, 135798. **[Impact Factor: 3.8]**

27. I Shafiq, I Amanat, M Khalid, **M A Asghar**, R Baby, S Ahmed, SM Alshehri "Influence of azo-based donor modifications on nonlinear optical amplitude of D-π-A based organic chromophores: A DFT/TD-DFT exploration" *Synthetic Metals*, 2023, 297, 117410. **[Impact Factor: 4.0]**

28. I. Shafiq, M.Khalid, M. Muneer , **M.A. Asghar*,** R. Baby, S. Ahmed, T. Ahamad, S. Figueirêdo de Alcântara Morais g, Ataualpa A.C. Braga "The impact of structural modifications into benzodithiophene compounds on electronic and optical properties for organic solar cells" *Materials Chemistry and Physics* 2023, 299,128154 **[Impact Factor: 4.778]**

29. M. Khalid, Z. Saeed, I. Shafiq, **M. A. Asghar**, A. A. C. Braga, S. M. Alshehri, M. S. Akram, S. C. Ojha "Designing Strategies towards Non-Fullerene DTCR1 Based Compounds for the Exploration of Non-linear Optical Behavior" *Journal of Saudi Chemical Society* 2023, 27, 101683. **[Impact Factor: 5.6]**

30. G. Mustafa, I. Shafiq, Q. Shaikh, A. Mustafa, R. Zahid, F. Rasool, **M. A. Asghar**, R. Baby, S. M. Alshehri, and M. Haroon "Quantum Chemical Exploration of A−π1–D1–π2–D2-Type Compounds for the Exploration of Chemical Reactivity, Optoelectronic, and Third-order Nonlinear Optical Properties" *ACS Omega* 2023, 8, 25, 22673–22683. **[Impact Factor: 4.132]**

31. S. Hussain, M. Adeel, M. Khalid, Ume Aiman, A. Villinger, A. A.C. Braga, S. M. Alshehri, **M. A. Asghar** "Efficient synthesis of nicotinaldehyde-based crystalline organic derivatives: Comparative analysis between experimental and DFT study" *Journal of Molecular Structure*, 2023, 1290, 135939. **[Impact Factor: 3.8]**

32. M. Khalid, S. Hanif, S. Ahmed, **M. A. Asghar,** M. Imran, A. A. C. Braga, S. C. Ojha "Exploration of nonlinear optical behavior in asymmetric dithieno [3,2b:2′,3′d] pyrrole based push pull constrain: A theoretical approach" *Journal of Saudi Chemical Society* 2023, 27, 101650. **[Impact Factor: 5.6]**

33. I. Shafiq, M. Khalid, **M. A. Asghar**, M. Adeel, M. F. Rehman, A. Syed, A. H Bahkali, A. M Elgorban, M. S. Akram "Exploration of photovoltaic behavior of benzodithiophene based non-fullerene chromophores: first theoretical framework for highly efficient photovoltaic parameters" *Journal of Materials Research and Technology*, 2023, 1882-1896. **[Impact Factor: 6.267]**

34. R. D. Alharthy, N. Ahmed, S. Mubarak, M. Yaqub, M. Khalid, I. Shafiq, **M. A. Asghar**, A. A. C. Braga, Z. Shafiq Design, "Synthesis, and Density Functional Theory Studies of Indole Hydrazones as Colorimetric "Naked Eye" Sensors for F Ions" *ACS Omega* 2023, 8, 15, 14131–14143. **[Impact Factor: 4.132]**

35. S. Bullo, R. Jawaria, I. Faiz, I. Shafiq, M. Khalid, **M. A. Asghar**, R. Baby, R. Orfali, S. Perveen "Efficient Synthesis, Spectroscopic Characterization, and Nonlinear Optical Properties of Novel Salicylaldehyde-Based Thiosemicarbazones: Experimental and Theoretical Studies" *ACS*

Omega 2023, 8, 15, 13982–13992. **[Impact Factor: 4.132]**

36. M. N. Tahir, A. Ali, M. Khalid, M. Ashfaq, M. Naveed, S. Murtaza, I. Shafiq, **M. A. Asghar**, R. Orfali, S. Perveen "Efficient Synthesis of Imine-Carboxylic Acid Functionalized Compounds: Single Crystal, Hirshfeld Surface and Quantum Chemical Exploration" *Molecules* 2023, 28(7), 2967. **[Impact Factor: 4.927]**

37. H. Mehmood, T. Akhtar, M. Haroon, M. Khalid, S. Woodward, **M. A. Asghar**, R. Baby, R. Orfali, S. Perveen "Synthesis of Fluorinated Hydrazinylthiazole Derivatives: A Virtual and Experimental Approach to Diabetes Management" *ACS Omega* , 2023, 8, 12, 11433–11446. **[Impact Factor: 4.132]**

38. OAA Ali, MU Khan, **MA Asghar**, SF Mahmoud, SM El-Bahy, R Baby "A new cyano (− CN) free molecular design perspective for constructing carbazole-thiophene based environmental friendly organic solar cells" *Physica B: Condensed Matter* 652, 414630. **[Impact Factor: 2.8]**

39. R. D Alharthy, I. Urooj, M. Tasleem, M. Khalid, **M. A. Asghar,** S. I. Khan, M. Ajmal, N. Ahmed, Z. Shafiq "Synthesis of novel 3-hydroxy-2-naphthoic hydrazones as selective chemosensors for cyanide ions" *RSC Advances*, 2023, 13,22, 15208-15221. **[Impact Factor: 4.036]**

40. M. Haroon, T. Akhtar, M. Khalid, H. Mehmood, **M. A. Asghar**, R. Baby, R. Orfali and S. Perveen "Synthesis, characterization and exploration of photovoltaic behavior of hydrazide based scaffolds: a concise experimental and DFT study" *RSC Advances*, 2023, 13, 7237. **[Impact Factor: 4.036]**

41. M. Khalid, U. Habiba, **M. A. Asghar**, M. Adeel, M. M. Alam, M. Imran, R. Baby, Ataualpa AC Braga, M. F. Rehman, M. S. Akram "Exploration of photovoltaic behavior of fused triphenylamine moiety as core donor with modified acceptors: Star-shaped D-π-A conjugated systems" *Materials Chemistry and Physics* 2023, 299,127528 **[Impact Factor: 4.778]**

42. M. U. Khan, R. Hussain, J. Yaqoob, M. F. Rehman, **M. A. Asghar,** S. D. Kanmazalp, M. A. Assiri, M. Imran, C. Lu, M. S. Akram "Theoretical design and prediction of novel fluorene-based non-fullerene acceptors for environmentally friendly organic solar cell" *Arabian Journal of Chemistry* 2023, 16, 104374. **[Impact Factor: 6.212]**

Year 2022

43. M. Khalid, R. Ahmed, I. shafiq, M. Arshad, **M. A. Asghar,** K. S. Munawar, M. Imran & A. A. C. Braga "First theoretical framework for highly efficient photovoltaic parameters by structural modification with benzothiophene-incorporated acceptors in dithiophene based chromophores" *Scientifc Reports* 2022, 12, 20148. **[Impact Factor: 4.996]**

44. M. Khalid, M. Zafar, S. Hussain, **M. A. Asghar**, R. A. Khera, M. Imran, F. Lhadi Abookleesh, M. Y. Akram, A. Ullah "Influence of End-Capped Modifications in the Nonlinear Optical Amplitude of Nonfullerene-Based Chromophores with a D−π–A Architecture: A DFT/TDDFT Study" *ACS Omega* 2022, 7, 27, 23532–23548. **[Impact Factor: 4.132]**

45. M. U. Khan, S. Hussain, **M. A. Asghar**, K. S. Munawar, R. A. Khera, M. Imran, M. Ibrahim, M. M Hessien, G. AM Mersal "Exploration of Nonlinear Optical Properties for the First Theoretical Framework of Non-Fullerene DTS(FBTTh2)2-Based Derivatives" *ACS Omega* 2022, 7, 21, 18027–18040. **[Impact Factor: 4.132]**

Year 2021

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