

CURRICULUM VITAE

Of

Khurshid Ayub, PhD, PostDoc (Canada)

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www.ctcrl.com (Personal)

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<http://sc.hec.gov.pk/aphds/submit.asp?supid=3966> (HEC)

<https://scholar.google.com.pk/citations?user=q0cqNi8AAAAJ&hl=en> (Google Scholar)

https://www.researchgate.net/profile/Khurshid_Ayub (Researchgate)

Areas of research

Computational chemistry, Single atom catalysis, Non-bonding interactions,
Photoswitches, Non-linear optical properties, Sensors, Adsorption/encapsulation,
Reactions in confined spaces, Singlet fission and Drug delivery

Personal

Date of Birth September 16, 1979
Place of Birth District Attock (Punjab, Pakistan)
CNIC # 37101-1692894-7

Theses Degrees

Ph.D University of Victoria, BC, Canada (January **2005** - December **2008**)
Thesis Title "The Synthesis, Thermal and Photochemical Properties of Cyclophanes and Dihydropyrenes with Different Internal Substituents"
M.Sc University of the Punjab, Lahore, Pakistan (September **1999** – March **2002**)

Thesis Title "Development of Phosphate Bath Based on Sodium Molybdate and Metal Cation"

Academic Record

Ph.D: Courses CGPA 8.43/9

GRE: 94 %ile, 2003 (ETS Princeton, USA)
(Chemistry)

M.Sc: (Chemistry)
Division: 1st (75.2%), University of the Punjab, Lahore, Pakistan. (Top position holder in the final year and the fifth position overall in the University)

B.Sc : Major Subjects: Chemistry, Zoology and Botany.
Division: 1st (67%), Govt. College Attock, University of the Punjab, Lahore, Pakistan. (Top position in the college)

H.S.S.C: Major Subjects: Chemistry, Biology, Physics.
Grade "A" (71%), Govt. College Attock, BISE Rawalpindi

SSC: Major Subjects: Chemistry, Biology, Physics and Mathematics.
Grade "A" (79%), Govt Boys High School F6RF PAC Kamra, BISE Rawalpindi

Awards and Scholarships

- 1. The Dr E. and Mrs. M Von Rudolf Award, Canada, (2005/06).**
- 2. Nora and Mark Degoutiere Memorial Scholarship, Canada, (2006/07).**
- 3. President Talent Award, Pakistan (2000-2001).**
- 4. Research Productivity Award, CIIT, Pakistan, (2011-2017).**
- 5. Research productivity Award from PCST, Pakistan (2011 (G), 2012 (D), 2013 (C), 2014 (B), 2015 (B), 2016 (B))**
- 6. Best Researcher Award, Department of Chemistry, CIIT, Abbottabad, Pakistan (2016)**
- 7. Campus Best Researcher Award, CIIT, Abbottabad, Pakistan (2017)**
- 8. Provincial Merit Award, Punjab, Pakistan (2000-2001).**
- 9. Distt. Attock Merit Scholarship, Punjab, Pakistan (1993-1994)**
- 10. Fauji Foudation Scholarship, Pakistan. (1998-2001).**
- 11. Benevolent Fund Scholarship, Punjab, Pakistan (1995-96, 1998-2001).**
- 12. Punjab Teacher Association Scholarship, Punjab, Pakistan (2000-01).**
- 13. DAAD Award (did not avail), Germany (2004).**

14. HEC Overseas Scholarship for Austria (did not avail) Pakistan, (2004).

Professional Experience

Date	Position	University
20 April 2018 - Present	Associate Professor	COMSATS University Islamabad, Abbottabad Campus, Pakistan
01 Sep 2013 - 14 July 2015	Assistant Professor	King Faisal University, Al- Ahsa, Saudi Arabia,
05 October 2010 - 19 April 2018	Assistant Professor	CIIT, Abbottabad Campus, Pakistan
01 January 2009 – 04 October 2010	Post-Doctoral Fellow	Queen's University, Kingston, ON, Canada
January 2011 - May 2011	Senior Warden SF Hostel	CIIT, Abbottabad Campus, Pakistan
01 June 2011 - 30 May 2012	Graduate Program Coordinator	Department of Chemistry, CIIT, Abbottabad Campus, Pakistan
01 January 2005 – 31 December 2007	Teaching Assistant	University of Victoria, Victoria, BC, Canada

Areas of interest

Research in my group is multidisciplinary but only through computational tools. We study a range of topics in chemistry. Currently the research projects are based on the following themes

1. Reactions in confined spaces
2. Non-bonding interactions
3. Transition metal catalysis.
4. Photoswitches, Photoswitchable catalysis.
5. Non-linear optical properties
6. Sensors
7. Adsorption/encapsulation
8. Single atom catalysis
9. Singlet fission
10. Drug delivery

Teaching

❖ COMSATS University Islamabad

20 April 2018 - Present

Abbottabad Campus, KPK, Pakistan

Associate Professor

- | | |
|---|------------------------------------|
| ❖ CIIT Abbottabad campus, KPK, Pakistan | 05 October 2010 - 19 April 2018 |
| Assistant Professor | |
| ❖ University of Victoria, B.C. Canada | 01 January 2005 - 31 December 2007 |
| Teaching Assistant | |

Highlights of Qualification

1. Experience in a range of DFT and *ab initio* methods of computational chemistry.
2. Experience with operating NMR 300, 400 & 500 MHz.
3. Experience with multinuclear NMR, FT-IR, GC-MS, UV-Vis and HPLC.
4. Experience with using POM, TGA, elemental analyzer and DSC.
5. Experienced in working with highly sensitive macromolecules, dihydropyrenes.

Administrative Responsibilities/Designation

- ❖ NMR handling and analysis
- ❖ Convener departmental grievances committee
- ❖ Thesis/synopsis quality evaluation
- ❖ Departmental evaluation committee
- ❖ Member Board of Studies, University of Kotli (Azad Jammu and Kashmir)

Session Chair (Conference)

1. *International Conference on Green and Sustainable Chemical Sciences*, Daud University of Engineering and Technology, Karachi 03-04 March 2018
2. *International Conference on Chemical Sciences*, Quaid-i-Azam University, Islamabad, 24-26 April 2019

Invited Talks

1. **University of Agriculture Faisalabad**
2. “*Understanding the Theoretical Models for Better Solving the Practical Problems in Chemical Sciences*” **1ST International Workshop on Hands on**

Training of Computational Software's in Chemistry, University of Bahrain, Bahrain

3. AJK

4. *“Exploration of Nonlinear Optical Materials through Computational Tools” 1st International Conference on Trends and Research in Chemistry, University of Education Lahore, January 18-19, 2022*
5. *“Strategies for Accuracy and Low Computational Cost” University of Wah, Wah, December 13, 2021*
6. *Understanding the Theoretical Models for Better Solving the Practical Problems in Chemical Sciences” COMSATS University Islamabad, Lahore Campus, November 11, 2021*
7. *“Understanding the Theoretical Models for Better Solving the Practical Problems in Chemical Sciences” University of Wah, Wah, August 25, 2021*
8. *“Permeation Selectivity of Alkali Metal Ions Through Crown Ether Based Synthetic Ion Channels” 3rd International Conference on Chemical and Pharmaceutical Sciences: New Trends in Medicinal and Pharmaceutical Chemistry. Forman Christian College University, Lahore, January 29-31, 2020.*
9. *“Rational Design Strategy and Non-linear Optical Response of Alkaline Earthides; A New Entry to Excess Electron Materials”. International Conference on Chemical Sciences, Quaid-i-Azam University Islamabad, 24-26 April 2019*
10. *“Understanding the Theoretical Models for Better Solving the Practical Problems in Chemical Sciences” 1st National workshop on Computational Chemistry and Drug Design, University of Science and Technology, Bannu, December 19-20, 2018*
11. *“Nonlinear Optical Response of Exohedral and Endohedral Alkali Metal Doped $X_{12}Y_{12}$ Nanoclusters” Modern Trends in Chemistry and Energy Technologies, COMSATS University, Lahore Campus, October 22-23, 2018*
12. *“Differential Permeability of Proton Isotopes through B and N Doped Graphene Membranes” International Conference on Green and Sustainable Chemical Sciences, Daud University of Engineering and Technology, 03-04 March 2018 (Keynote Speaker)*

13. ***“Alkalides and Metallides; Violating the General Design Principle”***. **3rd International Conference on “Recent Trends in Chemistry”** Allama Iqbal Open University, November 23-24, 2017
14. ***“Kinetics, Thermodynamics and Non-linear Optical Properties of Alkali Metal Doped $X_{12}Y_{12}$ Nano-cages”*** **National Center of Excellence in Physical Chemistry, University of Peshawar. December 01, 2016**
15. ***“Alkali Metal Doped Nano-structures: Efficient Non-linear Optical Materials”*** **2nd International Chemistry Conference: Recent Trends in Chemistry, Allama Iqbal Open University, Islamabad. November 24-25, 2016**
16. ***“Photoswitchable Frustrated Lewis Pairs: Potential Applicants in Controlled Hydrogenation homogeneous Catalysis and Hydrogen Storage”*** **COMSATS Institute of Information Technology, Abbottabad, October 28, 2015**
17. ***“Rational Design of de-Vries Like FLCs for Display Applications”*** **Tsinghua University, Beijing China, May 27, 2012**
18. ***“Chemistry with Limited Resources: Computational Chemistry. An Introduction of Molecular Dynamics”*** **Abdul Wali Khan University, Mardan, Pakistan. March 29, 2011.**
19. ***“Developing Rational Design Strategy for de Vries Like Liquid crystals”*** **Abdul Wali Khan University, Mardan, Pakistan. March 30, 2011.**

Resource person in workshops/conferences

1. ***“Introduction to Computational Chemistry and Drawing Tools”*** **2nd National Workshop on Basic Tools in Bioinformatics: Molecular Modeling, Government College University Lahore, March 07-08, 2019**
2. ***“Essential Computational Chemistry for Experimentalist using DFT”*** **2nd National Workshop on Basic Tools in Bioinformatics: Molecular Modeling, Government College University Lahore, March 07-08, 2019**
3. ***“Understanding the Theoretical Models for Better Solving the Practical Problems in Chemical Sciences”*** **1st National workshop on Computational Chemistry and Drug Designing, University of Science and Technology, Bannu, December 19-20, 2018**

4. “Modeling Reaction Intermediates and Transition States” *Computational Chemistry Workshop* A New Approach to Understanding and Solving Chemical Problems, Forman Christian College University, 20-22 January 2016.

Conference Talks

1. “Synthesis, Kinetics and NMR Properties of Cyclophanediene-Dihydropyrene Photoswitches”.(Opening talk) **Khurshid Ayub**, Reginald H. Mitchell. *VIVA II NMR Symposium, University of Victoria, June 20-21, 2008.*
2. “Design of “de Vries like” Liquid Crystals by Frustration between SmA and SmC Promoting Elements (Lecture)” **Khurshid Ayub**, Robert P Lemieux, Qingxiang Song, Jeffery C Roberts, Dorothee Nonnemacher, Nadia Kapernaum and Frank Giesselmann. *9th International and 21st National Chemistry Conference, University of Karachi, Karachi, Pakistan, February 7-9 2011,*
3. “Mesogenic Dopants Based on Axially Chiral Dinitrobiphenyl Core” **Khurshid Ayub** and Robert P. Lemieux., *93rd Canadian Chemistry Conference and Exhibition, Toronto May 29 – June 2, 2010..*
4. “An Accurate Cost Effective DFT Approach to Study the Sensing Behavior of Polypyrrole Towards Nitrate Ion in Gas and Aqueous Phases” Fatima Wasim, Tariq Mahmood, **Khurshid Ayub**, *14th EurAsia Chemistry Conference, University of Karachi, Karachi, Pakistan, December 15-18, 2016,*

Publications

2022

1. Insighting the Inhibitory Potential of Novel Modafinil Drug Derivatives Against Estrogen Alpha ($ER\alpha$) of Breast Cancer Through a Triple Hybrid Methodology, Afsheen Saba, Fatima Sarwar, Shabbir Muhammad, Mubasshar Ilyas, Javed Iqbal, Abdullah G. Al-Sehemi, **Khurshid Ayub**, Mazhar Amjad Gilani, Muhammad Adnan, *Journal of Molecular Liquids*, 2022, Accepted (**IF = 6.633**)
2. Insighting the nonlinear optical (NLO) response of pure Au_m ($2 \leq m \leq 7$) and copper doped $Au_{m-x}Cu_x$ clusters, Fakhar Hussain, Riaz Hussain, Muhammad Adnan, Shabbir Muhammad, Zobia Irshad, Muhammad Usman Khan, Junaid Yaqoob, **Khurshid Ayub**, *RSC Advances*, 2022, Accepted (**IF = 4.036**)
3. Structure and electronic characterization of pristine and functionalized single wall carbon nanotube interacting with sulfide ion: A density functional theory approach Sania Bibi, Sehrish Sarfaraz, Muhammad Yar, Muhammad Iqbal

Zaman*, Abdul Niaz, Ayesha Khan, Muhammad Ali Hashmi, & **Khurshid Ayub***, *Journal of Molecular Liquids*, **2022**, Accepted (IF = 6.633)

4. Surface Functionalization of Si₆Li₆ Cluster with Superalkalis to Achieve High Nonlinear Optical Response: A DFT Study, Faiqa Khaliq, Aqsa Afzaal, Sobia Tabassum, Tariq Mahmood, **Khurshid Ayub**, Asim Laeeq Khan, Muhammad Yasin and Mazhar Amjad Gilani, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2022**, 653, 129985 (IF = 5.518)
5. Benzimidazole bearing thiourea analogues: Synthesis, β -glucuronidase inhibitory potential and their molecular docking study, Hayat Ullah, Hussan Zada, Fahad Khan, Shawkat Hayat, Fazl Rahim, Amjad Hussain, Amina Manzoor, Abdul Wadood, **Khurshid Ayub**, Ashfaq Ur Rehman, Sehrish Sarfaraz, *Journal of Molecular Structure*, **2022**, 1270, 133941 (IF = 3.841)
6. Role of Novel Carbon-Oxygen-Bridged Z-Shaped Non-Fullerene Acceptors for High Efficiency Organic Solar Cells, Riaz Hussain, Muhammad Adnan, Saba Nawab, Muhammad Usman Khan, Muhammad Khalid, Zobia Irshad, **Khurshid Ayub**, Jongchul Lim *Synthetic Metals*, **2022**, Accepted, 290, 117159 (IF = 4.0)
7. Organic transformations in the confined space of porous organic cage CC2: A DFT study, Ayehsa Mukhtar, Sehrish Sarfaraz, **Khurshid Ayub***, *RSC Advances*, **2022**, 12, 24397–24411 (IF = 4.036)
8. ON-OFF” NLO switch based on coordination complexes of iron and cobalt containing isomeric ligand: A DFT study, Tamseela Bibi, Tabish Jadoon and **Khurshid Ayub***, *RSC Advances*, **2022**, 12, 23204–23214 (IF = 4.036)
9. DFT study of super-halogen (Al₇) doped graphitic carbon nitride (C₂N) and its nonlinear optical properties, 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 (IF = 3.841)
10. Mechanochemical Ni-catalysed arylation of ortho-hydroxyarylenaminones: Synthesis of isoflavones Satenik Mkrtchyan, Michal Jakubczyk, Suneel Lanka, Muhammad Yar, Tariq Mahmood, **Khurshid Ayub**, Mika Sillanpaa, Christine Thomas, Viktor Iaroshenko, *Advanced Synthesis & Catalysis*, **2022**, Accepted (IF = 5.981)
11. Molecular docking, dynamics, and quantum chemical study of vanillylacetone and beta-hydroxy ketone derivatives against M_{pro} of SARS-CoV-2, Saniyah Amin, Shabbir Muhammad, Javed Iqbal, Sami Ullah, Abdullah G. Al-Sehemi, H. Algarni, Saleh S Alarfaji, and **Khurshid Ayub**, *South African Journal of Chemistry*, **2022**, 76, Accepted (IF = 1.286)
12. Superhalogen doping of aromatic heterocycles; effective approach for the enhancement of static and dynamic NLO response, Misbah Asif, Hasnain Sajid, Mazhar Amjad Gilani, **Khurshid Ayub** and Tariq Mahmood, *Vacuum*, **2022**, 203, 111301 (IF = 4.11)

13. Enhanced Non-Linear Optical Response of Alkali Metal-Doped Nitrogenated Holey Graphene (C₂N) | Wishah Akram; Emaan Nadeem; **Khurshid Ayub**, Javed Iqbal, M. S. Al-Buriahi; Sultan Alomairy; Khadijah Mohammedsahleh Katubi, Awad A. Ibraheem, *Journal of Molecular Structure* **2022**, 1267, 133580 (IF = 3.841)
14. Theoretical Investigation of Lithium-based clusters Li_n (where n=3, 5, 7) with remarkable electronic and frequency-dependent NLO properties, Atazaz Ahsin and **Khurshid Ayub***, *European Physical Journal Plus*, **2022**, 137: 803 (IF = 3.758)
15. Alkaline earth metals doped C₂N with Enhanced non-linear optical properties, Emaan Nadeem, Wishah Akram, Rao Aqil Shehzad, **Khurshid Ayub**, Javed Iqbal, Asma M Alenad, T.A. Taha, *Optik*, **2022**, 265, 169514 (IF = 2.84)
16. Lanthanum Doped Corannulenes with Enhanced Static and Dynamic Nonlinear Optical Properties: A First Principle Study, Rehana Bano, Sabir Hussain, Muhammad Arshad, Abdur Rauf, Tariq Mahmood, **Khurshid Ayub**, Mazhar Amjad Gilani, *Physica B: Condensed Matter*, **2022**, 641, 414088 (IF = 2.988)
17. Benchmark DFT approach for the calculation of bond dissociation energies of the M-O₂ bond: a key step in water splitting reactions. Naveen Kosar, **Khurshid Ayub**, Mazhar Amjad Gilani, Shabbir Muhammad and Tariq Mahmood, *ACS Omega*, **2022**, 7, 24, 20800-20808 (IF = 4.132)
18. DFT study of transition metal doped calix-4-pyrrole with excellent electronic and nonlinear optical properties, Areeba Asif, Nimra Maqsood, Zainab Mufarreh Elqahtani, **Khurshid Ayub**, Muhammad Ans, Javed Iqbal, M.S. Al-Buriahi, Sultan Alomairy, Z.A.Alrowaili, *Computational and Theoretical Chemistry*, **2022**, 1214, 113767 (IF = 2.292)
19. Computation Assisted Design and Prediction of Alkali-Metal-Centered B₁₂N₁₂ Nanoclusters for Efficient H₂ Adsorption: New Hydrogen Storage Materials, Muhammad Yasir Mehboob, Riaz Hussain, Faiza Younas, Saba Jamil, Malik Muhammad Asif Iqbal, **Khurshid Ayub**, Nargis Sultana, Muhammad Ramzan Saeed Ashraf Janjua, *Journal of Cluster Science*, **2022**, Accepted (IF = 3.447)
20. Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19, Muhashar Ilyas, Shabbir Muhammad, Javed Iqbal, Saniyah Amin, Abdullah G Al-sehemi, H. Algarni, Saleh S Alarfaji, Muhammad Y. Alshahrani, **Khurshid Ayub**, *Chemical Papers*, Accepted **2022**, (IF = 2.146)
21. DFT Based modeling of Asymmetric non-fullerene acceptors for high-performance organic solar cell, Noureen Kanwal, Riaz Hussain, Abdul Sattar, Mohammed A, Assiri, Muhammad Imran, Ajaz Hussain, Mirza Arfan Yawer, Riaz Hussain, Muhammad Yasir Mehboob, Muhammad Khalid, **Khurshid Ayub** and Talha Hassan, *Optical and Quantum Electronics*, **2022**, 54:546 (IF 2.794)
22. *Ab-initio* study for superior sensitivity of graphyne nanoflake towards nitrogen halides over ammonia, Hasnain Sajid, Sidra Khan, **Khurshid Ayub**, Mazhar Amjad Gilani, Tariq Mahmood, Umar Farooq, Muhammad Salim Akhtar, *Journal of Molecular Modeling*, **2022**, 28:161 (IF = 2.172)

23. Hetero-Porphyrin based Channel for Separation of Proton Isotope: A Density Functional Theory Study Amna Ayub, **Khurshid Ayub***, Sehrish Gul, Muhammad Ali Hashmi, Ahmed Lakhani, Saleem Iqbal, Javed Iqbal, *Microporous and Mesoporous Materials*, **2022**, 339, 111995 (IF = 5.876)
24. Static, dynamic nonlinear optical (NLO) response and electrider characteristics of superalkalis doped star like $C_6S_6Li_6$, Naveen Kosar, Laraib Zari, **Khurshid Ayub**, Mazhar Amjad Gilani and Tariq Mahmood, *Surfaces and Interfaces*, **2022**, 31, 102044 (IF = 6.137)
25. Mixed superalkalis are better choice than pure superalkalis for $B_{12}N_{12}$ nanocage to design high performance nonlinear optical materials. Rehana Bano, **Khurshid Ayub**, Tariq Mahmood, Muhammad Arshad, Ahsan Sharif, Sobia Tabassum, Mazhar Amjad Gilani, *Dalton Transactions*, **2022**, 51, 8437-8451 (IF = 4.569)
26. Adsorption of industrial gases (CH_4 , CO_2 and CO) on olympicene: A DFT and CCSD(T) investigation, Uroosa Sohail, Faizan Ullah, Tariq Mahmood, Shabbir Muhammad and **Khurshid Ayub***, *ACS Omega*, **2022**, 7(22), 18852-18860 (IF = 4.132)
27. DFT study of alkali and alkaline earth metals doped benzocryptand with remarkable NLO properties Nimra Maqsood, Areeba Asif, **Khurshid Ayub**, Javed Iqbal, Ashraf Y. Elnaggar, Gaber A. M. Mersal, Mohamed M. Ibrahim, Salah M. ElBahy, *RSC Advances* **2022**, 12, 16029-16045 (IF = 4.036)
28. Enhancement of NLO properties of supersalt ($Al(BH_4)_3$)-doped graphene: a DFT study. Humera, Ijaz Ahmad Bhatti, Muhammad Mohsin, Nyla Amjad, Rao Aqil Shehzad, **Khurshid Ayub**, Javed Iqbal, T A Taha, *Journal of Molecular Modeling*, **2022**, 28: 164 (IF = 2.172)
29. A quantum chemical study of outstanding structural, electronic and nonlinear optical polarizability of boron nitride ($B_{12}N_{12}$) doped with super salt (P_7BaNO_3). Ali Raza Ayub, Umar Yaqoob, Sidra Rafiq, Rao Aqil Shehzad, **Khurshid Ayub**, Javed Iqbal, Hui Li, K. H. Mahmoud, Khalid A Elsayed, *Journal of Inorganic and Organometallic Polymers and Materials*, **2022**, Accepted (IF = 3.518)
30. Theoretical investigation of double-cubed polycationic cluster ($Sb_7Se_8Cl_2$)³⁺ for the storage of helium and neon. Maryam Munir, Faiza Ahsan, Muhammad Yar, **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2022**, 148, 106756 (IF = 4.644)
31. Selective electrochemical sensing of formaldehyde over thioformaldehyde, phosgene and thiophosgene by using h-g- C_3N_4 nanoflake, Sana Qureshi, Misbah Asif, Hasnain Sajid, Mazhar Amjad Gilani, Khurshid Ayub, Muhammad Arshad, Tariq Mahmood, *Materials Science in Semiconductor Processing*, **2022**, 148, 106753 (IF = 4.644)
32. Nonlinear Optical Response of 9,10-bis(phenylethynyl)anthracene mediated by electron donating and electron withdrawing substituents: A Density Functional Theory approach. Faiz Rasool, Ajaz Hussain, Muhammad Yar, **Khurshid Ayub**, Muhammad

- Sajid, Muhammad Ali Khan, Hafiz Muhammad Asif, Muhammad Imran, Mohammed A. Assiri, *Materials Science in Semiconductor Processing*, **2022**, 148, 106751 (IF = 4.644)
33. Remarkable non-linear optical properties of gold cluster doped graphyne (GY): A DFT study, Alvina Rasool, Saba Zahid, Nada Alfryyan, Ali Raza Ayub, **Khurshid Ayub**, Mohammed Salim Akhtar, Javed Iqbal, M.S. Al Buriahi, El Sayed Yousef, *Journal of Molecular Graphics and Modelling*, **2022**, 114, 108204 (IF = 2.942)
 34. Non-fullerene near-infrared sensitive acceptors "Octacyclic naphtho [1,2-b:5,6-b] dithiophene core" for organic solar cell applications: In Silico Molecular engineering, Abdul Sattar, Riaz Hussain, Sahar Ishaq, Mohammed A. Assiri, Muhammad Imran, Ajaz Hussain, Mirza Arfan Yawer, Saleem Jan, Riaz Hussain, Muhammad Yasir Mehboob, Muhammad Khalid, **Khurshid Ayub**, *ACS Omega*, **2022**, 7, 16716-16727 (IF = 4.132)
 35. DFT study of the possible reaction path for radical promoted esterification mechanism of free fatty acids of walnut oil for the production of biodiesel. Naila Ghani, Naveen Kosar, Sana Sadaf, Tariq Mahmood, Muhammad Khalid, **Khurshid Ayub***, Javed Iqbal and Sadia Noor, *Letters in Organic Chemistry*, **2022**, Accepted (IF = 0.797)
 36. Synergistic end-capped engineering on non-fused thiophene ring based acceptors to enhance the photovoltaic properties of organic solar cells Ehsan Rashid, Javed Iqbal, Muhammad Khan, Yaser El-Badry, **Khurshid Ayub***, Rasheed Ahmad Khera, *RSC Advances*, **2022**, 12, 12321-12334 (IF = 4.036)
 37. Assessment of alkali/alkaline-earth metals doped cubanes as high performance nonlinear optical materials by first-principles study, Javeria Naeem, Rehana Bano, **Khurshid Ayub**, Tariq Mahmood, Sobia Tabassum, Mazhar Amjad Gilani, *Journal of Science: Advanced Materials and Devices*. **2022**, 7, 100457 (IF = 7.382)
 38. Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%. Rao Aqil Shehzad, **Khurshid Ayub**, M.S. Al-Buriahi, Nada Alfryyan, H.H. Somaily, Sultan Alomairy, Javed Iqbal. *Solar Energy*, **2022**, 237, 96-107 (IF = 7.188)
 39. Shedding Light on the Second Order Nonlinear Optical Responses of Commercially Available Acidic Azo Dyes for Laser Applications, Muhammad Fahad Asif, Rehana Bano, Robina Farooq, Shabbir Muhammad, Tariq Mahmood, Khurshid Ayub, Sobia Tabassum, Mazhar Amjad Gilani, *Dyes and Pigments*, **2022**, 202, 110284 (IF = 5.122)
 40. First-principles study for electrochemical sensing of neurotoxin hydrazine derivatives via h-g-C₃N₄ quantum dot. Sana Qureshi, Misbah Asif, Hasnain Sajid, Mazhar Amjad Gilani, **Khurshid Ayub**, Tariq Mahmood, *Surfaces and Interfaces*, **2022**, 30, 101913 (IF = 6.137)
 41. Sensing behaviour of monocyclic C₁₈ and B₉N₉ analogues toward chemical warfare agents (CWAs); quantum chemical approach Hasnain Sajid, **Khurshid Ayub**, Tariq Mahmood, *Surfaces and Interfaces*, **2022**, 30, 101912 (IF = 6.137)

42. DFT studies on electrochemical properties of halide ions doped GDY-28 nanoflake for Na-ion battery applications. Tayyaba Murtaza, Naveen Kosar, Mazhar Amjad Gilani, **Khurshid Ayub**, Khizar Hussain Shah and Tariq Mahmood, *Materials Science in Semiconductor Processing*, **2022**, 145, 106651 (IF = 4.644)
43. First principles calculations of the adsorption of fluorouracil and nitrosourea on CTF-0; organic frameworks as drug delivery systems for cancer treatment. Faiza Fayyaz, Muhammad Yar, Adnan Gulzar, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2022**, 356, 118941 (IF = 6.633)
44. Ab Initio Study of 2-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells. Saim Riaz, Riaz Hussain, Muhammad Adnan, Muhammad Usman Khan, Shabbir Muhammad, Junaid Yaqoob, Muhammad Usman Alvi, Muhammad Khalid, Zobia Irshad, **Khurshid Ayub**, *ACS Omega*, **2022**, 7, 10638-10648 (IF = 4.132)
45. Olympicene as a high-performance sensor for lung irritants: A dispersion corrected DFT insight. Uroosa Sohail, Faizan Ullah, Tariq Mahmood, **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2022**, 144, 106620 (IF = 4.644)
46. Enhancement in non-linear optical properties of carbon nitride (C₂N) by doping with superalkali (Li₃O): A DFT study. Talha Ishfaq, Rasheed Ahmad Khera, Saba Zahid, Umer Yaqoob, Rao Aqil Shehzad, **Khurshid Ayub** and Javed Iqbal, *Computational and Theoretical Chemistry*, **2022**, 1211, 113654 (IF = 2.292)
47. Quantum chemical designing of novel fullerene-free acceptor molecules for organic solar cell applications, Saira Khan, Riaz Hussain, Abdul Satar, Mohammed A. Assiri, Muhammad Imran, Ajaz Hussain, Mirza Arfan Yawer, Riaz Hussain, Muhammad Yasir Mehboob, Sajjad Hussain Sumra, Muhammad Khalid, **Khurshid Ayub**, *Journal of Molecular Modeling*, **2022**, 28:67 (IF = 2.172)
48. First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D- π -A configured optoelectronic materials for bulk heterojunction solar cell, Muhammad Yasir Mehboob, Muhammad Usman Khan, Riaz Hussain, Muhammad Khalid, Junaid Yaqoob, Rafia Rehman, Muhammad Bilal Ahmed Siddique, Muhammad Mujahid Alam, Muhammad Imran and **Khurshid Ayub**, *Physica B. Condensed Matter*, **2022**, 633, 413769 (IF = 2.988)
49. Potential sensing of toxic chemical warfare agents (CWA) by twisted nanographenes: A first principle approach, Naila Sattar, Hasnain Sajid, Sobia Tabassum, **Khurshid Ayub**, Tariq Mahmood, Mazhar Amjad Gilani, *Science of the Total Environment*, **2022**, 824, 153858 (IF = 10.753)
50. Therapeutic potential of C₂N as targeted drug delivery system for fluorouracil and nitrosourea to treat cancer: A theoretical study. Faiza Ahsan, Muhammad Yar, Adna Gulzar, **Khurshid Ayub***, *Journal of Nanostructure in Chemistry*, **2022**, Accepted (IF = 8)

51. M@[12-crown-4] and M@[15-crown-5] where (M=Li, Na, and K); The very first examples of non-conventional one alkali metal-containing alkalides with remarkable static and dynamic NLO response, Atazaz Ahsin, **Khurshid Ayub***, *Physica E*, **2022**, *140*, 115170 (IIF = **3.369**)
52. DFT investigation of adsorption of nitro-explosives over C₂N surface: Highly selective towards trinitro benzene, Sehrish Sarfaraz, Muhammad Yar, Adnan Ali Khan, Rashid Ahmed, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2022**, *352*, 118652 (IF = **6.633**)
53. Optimized Nonlinear Optical (NLO) Response of Silicon Carbide Nanosheet by Alkali Metals Doping: A DFT Insight. Junaid Yaqoob, Tariq Mahmood, **Khurshid Ayub**, Sobia Tabassum, Ather Farooq Khan, Shagufta Perveen, Jucai Yang and Mazhar Amjad Gilani, *European Physical Journal Plus*, **2022**, *137*:233 (IF = **3.758**)
54. Silver cluster doped graphyne (GY) with outstanding non-linear optical properties, Saba Zahid, Alvina Rasool, Ali Raza Ayub, **Khurshid Ayub**, Javed Iqbal, M. S. Al-Buriahi, Norah Alwadai , H. H. Somaily, *RSC Advances*, **2022**, *12*, 5466-5482 (IF = **4.036**)
55. Superalkali (Li₂F, Li₃F) doped Al₁₂N₁₂ electride with enhanced static and dynamic nonlinear optical responses and refractive indices, Rehana Bano, Muhammad Arshad, Tariq Mahmood, **Khurshid Ayub**, Ahsan Sharif, Sobia Tabassum, Mazhar Amjad Gilani, *Materials Science in Semiconductor Processing*, **2022**, *143*, 106518 (IF = **4.644**)
56. Highly accurate DFT investigation for triggering the ultra-strong static and dynamic nonlinear optical properties of superalkali doped aminated graphdiyne (NH₂-GDY) donor- π -acceptor (D- π -A) quantum dots. Misbah Asif, Hasnain Sajid, **Khurshid Ayub**, Mazhar Amjad Gilani, Tariq Mahmood, *Polyhedron*, **2022**, *215*, 115695 (IF = **2.975**)
57. Shedding light on the optical and nonlinear optical properties of superalkali-doped borophene, Muhammad Hussnain, Rao Aqil Shehzad, Shabbir Muhammad, Javed Iqbal, Abdullah G. Al-Sehemi, Saleh S. Alarfaji, **Khurshid Ayub** and Muhammad Yaseen, *Journal of Molecular Modeling*, **2022**, *28*:46 (IF = **2.172**)
58. Computational investigation of a covalent triazine framework (CTF-O) as an efficient electrochemical sensor, Sehrish Sarfaraz, Muihammad Yar, Muhammad Ans, Mazhar Amjad Gilani, Ralf Ludwig, Muhammad Ali Hashmi, Masroor Hussain, Shabbir Muhammad and **Khurshid Ayub***, *RSC Advances*, **2022**, *12*, 3909-3923 (IF = **4.036**)
59. Permeability of boron- and nitrogen-doped graphene nanoflakes for protium/deuterium ions, Iram Gul, Muhammad Yar, Arsalan Ahmed, Muhammad Ali Hashmi and **Khurshid Ayub***, *RSC Advances*, **2022**, *12*, 2882-2891 (IF = **4.036**)

60. Enhanced non-linear optical response of Calix[4]pyrrole complexant based earthides in the presence of oriented external electric field, Annum Ahsan, Sehrish Sarfaraz, Faiza Fayyaz, Maria Asghar, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2022**, 350, 118504 (IF = 6.633)
61. Bithieno Thiophene-Based Small Molecules for Application as Donor Materials for Organic Solar Cells and Hole Transport Materials for Perovskite Solar Cells, Alvina Rasool, Saba Zahid, Muhammad Ans, Shabbir Muhammad, **Khurshid Ayub** and Javed Iqbal, *ACS Omega*, **2022**, 7, 1, 844-862 (IF = 4.132)
62. Experimental and Theoretical investigations on (E)-3-(4-ethoxyphenyl)-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-one and (E)-3-(naphthalen-2-yl)-1-(2-(trifluoromethyl) phenyl)prop-2-en-1-one: DNA binding, Urease inhibition and Promising NLO response, Faiz Rasool, Ajaz Hussain, **Khurshid Ayub**, Muahmmad Tariq, Khalid Mahmood, Sammer Yousuf, Muhammad Yar, Muhammad Khalid, Hafiza Saba Samreen, Mehreen Lateef and Abdul Malik, *Journal of Molecular Structure*, **2022**, 1253, 132194 (IF = 3.841)
63. Theoretical approach to evaluate the gas-sensing performance of graphene nanoribbon/oligothiophene composites, Ayesha Ashraf, John M. Herbert, Shabbir Muhammad, Bilal Ahmad Farooqi, Umar Farooq, Muhammad Salman and **Khurshid Ayub***, *ACS Omega*, **2022**, 7, 2, 2260-2274 (IF = 4.132)
64. Germanium-based superatom clusters as excess electron compounds with significant static and dynamic NLO response; A DFT study. Atazaz Ahsin, Ahmed Bilal Shah and **Khurshid Ayub***, *RSC Advances*, **2022**, 12, 365-377 (IF = 4.036)
65. Covalent triazine framework (CTF-0) surface as a smart sensing material for the detection of CWAs and industrial pollutants. Sehrish Sarfaraz, Muhammad Yar, **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2022**, 139, 106334 (IF = 4.644)
66. Nano-porous C₄N as a toxic pesticide's scavenger: A quantum chemical approach. Misbah Asif, Hasnain Sajid, **Khurshid Ayub**, Adnan Ali Khan, Rashid Ahmad, Muhammad Ans, Tariq Mahmood, *Journal of Molecular Graphics and Modelling*, **2022**, 108078 (IF = 2.942)
67. DFT study of OLi₃ and MgF₃ Doped Boron Nitride with Enhanced Nonlinear Optical Behavior. Saqib Shafiq, Rao Aqil Shehzad, Muhammad Yaseen, **Khurshid Ayub**, Ali Raza Ayub, Javed Iqbal, Khaled H.Mahmoud, Zeinhom M. El-Bahy, *Journal of Molecular Structure*, **2022**, 1253, 131934 (IF= 3.841)
68. Remarkable nonlinear optical response of Mn@C₂₀ (M = Na & K and n = 1–6); a DFT outcome. Naveen Kosar, Hira Tahir, **Khurshid Ayub**, Mazhar Amjad Gilani, Muhammad Imran, Tariq Mahmood, *Materials Science in Semiconductor Processing*, **2022**, 138, 106269 (IF = 4.644)

69. Superalkali-based alkalides $\text{Li}_3\text{O}@[12\text{-crown-4}]\text{M}$ (where M= Li, Na, and K) with remarkable static and dynamic NLO properties; A DFT study. Atazaz Ahsin, **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2022**, 138, 106524 (IF = 4.644)
70. Face specific doping of Janus all-*cis*-1,2,3,4,5,6-hexafluorocyclohexane with superalkalis and alkaline earth metals leads to enhanced static and dynamic NLO responses, Rehana Bano, Muhammad Arshad, Tariq Mahmood, **Khurshid Ayub**, Ahsan Sharif, Shagufta Perveen, Sobia Tabassum, Jucai Yang, Mazhar Amjad Gilani, *Journal of Physics and Chemistry of Solids*, **2022**, 160, 110361 (IF = 4.383)
71. A first principles study on electrochemical sensing of highly toxic pesticides by using porous C₄N nanoflake, Misbah Asif, Hasnain Sajid, **Khurshid Ayub**, Muhammad Ans and Tariq Mahmood, *Journal of Physics and Chemistry of Solids*, **2022**, 160, 110345 (IF = 4.383)
72. Permeation selectivity of pristine and vacancy defected hexagonal boron membranes for alkaline earth metal and ions, Sajida Munsif, **Khurshid Ayub***, *Journal of Biomolecular Structure and Dynamics*, **2021**, accepted (IF = 5.235)
73. Remarkable electronic and NLO properties of bimetallic superalkali clusters: A DFT study, Atazaz Ahsin, **Khurshid Ayub***, *Journal of Nanostructure in Chemistry*, **2022**, 12, 529-545 (IF = 8.0)

2021

74. Novel Star-Shaped Benzotriindole-Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for High-Performance Organic Solar Cells , Arooza Rafiq, Riaz Hussain, Muhammad Usman Khan, Muhammad Yasir Mehboob, Muhammad Khalid, Shehnaz, Mohammed Mujahid Alam, Muhammad Imran, **Khurshid Ayub**, *Energy Technology*, **2021**, 2100751 (IF =3.631)
75. A Theoretical Perspective on Strategies for the Fabrication of High Performance Nonlinear Optical Materials. Rehana Bano, Maria Asghar, **Khurshid Ayub**, Tariq Mahmood, Javed Iqbal, Sobia Tabassum, Rozalina Zakaria, Mazhar Gilani, *Frontiers in Materials*, **2022**, 8, 783239 (IF = 3.985)
76. Novel microporous B₆N₆ covalent organic framework (COF) as an electrochemical sensor for the ultra-selective detection of nitroaniline isomers; a DFT outcome, Hasnain Sajid, Misbah Asif, **Khurshid Ayub**, Mazhar Amjad Gilani, Mohammed Salim Akhter, Tariq Mahmood, *Surfaces and Interfaces*, **2021**, 27, 101587 (IF = 6.137)
77. Demonstrating the Potential of Alkali Metal-Doped Cyclic C₆O₆Li₆ Organometallics as Electrified and High-Performance NLO Materials, Sunaina Wajid, Naveen Kosar, Faizan Ullah, Mazhar Amjad Gilani, **Khurshid**

Ayub, Shabbir Muhammad, Tariq Mahmood, *ACS Omega*, **2021**, 6, 44, 29852–29861
(**IF = 4.132**)

- 78.** Exploring the interaction of ionic liquids with Al₁₂N₁₂ and Al₁₂P₁₂ nanocages for better electrode-electrolyte materials in super capacitors Palwasha Khan, Muhammad Jamshaid, Sobia Tabassum, Shagufta Perveen, Tariq Mahmood, Khurshid Ayub, Jucai Yang, Mazhar Amjad Gilani, *Journal of Molecular Liquids*, **2021**, 344, 117828 (**IF= 6.633**)
- 79.** C₁₀F as a potential anode material for alkali-ion batteries; a quantum chemical approach. Faizan Ullah. **Khurshid Ayub** Mazhar Amjad Gilani, Muhammad Imran, Tariq Mahmood, *Computational and Theoretical Chemistry*, **2021**, 1206, 113470 (**IF = 2.292**)
- 80.** Mechanochemical Transformation of CF₃ Group: Synthesis of Amides and Schiff Bases. Satenik Mkrtchyan, Michal Jakubczyk, Suneel Lanka, Muhammad Yar, **Khurshid Ayub**, Mohanad Shkooor, Michael Pittelkow, Viktor O. Iaroshenko, *Advanced Synthesis & Catalysis*, **2021**, 363, 1-14 (**IF = 5.981**)
- 81.** Extremely large static and dynamic nonlinear optical response of small superalkali clusters NM₃M' (M, M'=Li, Na, K), Atazaz Ahsin, **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*. **2021**, 109 108031 (**IF = 2.942**)
- 82.** High performance SACs for HER process using late first-row transition metals anchored on graphyne support: A DFT insight. Faizan Ullah, **Khurshid Ayub** and Tariq Mahmood, *International Journal of Hydrogen Energy*, **2021**, 46, 37814-37823 (**IF = 7.132**)
- 83.** Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties Amna Bibi, Shabbir Muhammad, Shafiq-ur Rehman, Shamsa Bibi, Shahid Bashir, **Khurshid Ayub**, Muhammad Adnan, and Muhammad Khalid, *ACS Omega*, **2021**, 6, 24602-24613 (**IF = 4.132**)
- 84.** Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications Mahira Rafiq, Rasheed Ahmad Khera, Maham Salim, Muhammad Khalid, **Khurshid Ayub**, Javed Iqbal. *Chemical Physics Letters*. **2021**, 782, 139018 (**IF = 2.7198**)
- 85.** Adsorption mechanism of p-aminophenol over silver graphene composite: A first principles study. Tabish Jadoon, Atazaz Ahsin, Faizan Ullah, Tariq Mahmood, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2021**, 341, 117415 (**IF = 6.633**)
- 86.** Electrochemical sensing behavior of graphdiyne nanoflake towards uric acid: a quantum chemical approach. Misbah Asif, Hasnain Sajid, **Khurshid Ayub**, Mazhar Amjad Gilani, Muhammad Salim Akhter and Tariq Mahmood, *Journal of Molecular Modeling*, **2021**, 27: 244 (**IF = 2.172**)

87. First example of lanthanum as dopant on $\text{Al}_{12}\text{N}_{12}$ and $\text{Al}_{12}\text{P}_{12}$ nanocages for improved electronic and nonlinear optical properties with high stability Faiqa Khaliq, **Khurshid Ayub**, Shabbir Muhammad, Tariq Mahmood, Sobia Tabassum, Mazhar Amjad Gilani, *Materials Science in semiconductor Processing*, **2021**, 135, 106122 (IF = 4.644)
88. Impact of even number of alkaline earth metal doping on the NLO response of C_{20} nanocluster; a DFT outcome Naveen Kosar, Hira Tahir, **Khurshid Ayub**, Mazhar Amjad Gilani, Muhammad Arshad, Tariq Mahmood *Computational and Theoretical Chemistry*, **2021**, 1204, 113386 (IF = 2.292)
89. Synthesis, characterization, antimicrobial, cytotoxic, DNA-interaction, molecular docking and DFT studies of novel di- and tri-organotin(IV) carboxylates using 3-(3-nitrophenyl)2-methylpropenoic acid, Muhammad Tariq, Rabbia Khan, Ajaz Hussain, Atia Batool, Faiz Rasool, Muhammad Yar, **Khurshid Ayub**, Muhammad Sirajuddin, Faizan Ullah, Saqib Ali, Arusa Akhtar, Samia Kausar, Ataf Ali Altaf, *Journal of Coordination Chemistry*, **2021**, 74, 2407-2426 (IF = 1.869)
90. A theoretical framework of Zinc decorated inorganic $\text{Mg}_{12}\text{O}_{12}$ nanoclusters for efficient COCl_2 adsorption: A step forward towards development of COCl_2 sensing materials Shahid Hussain, Shahzad Ali Shahid Chatha, Abdullah Ijaz Hussain, Riaz Hussain, Muhammad Yasir Mehboob, Asim Mansha, Nabeel Shahzad, **Khurshid Ayub***, *ACS Omega*, **2021**, 6, 19435-19444 (IF = 4.132)
91. Second-order NLO properties and two-state switching effects of transition metal redox complexes of iron and cobalt: A DFT study, Tamseela Bibi, Tabish Jadoon, Shabbir Muhammad, **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107975 (IF = 2.942)
92. Tuning the optoelectronic properties of superalkali doped phosphorene, Ayesha Hanif, Rida Kiran, Rasheed Ahmad Khera, Ayesha Ayoub, **Khurshid Ayub** and Javed Iqbal, *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107973 (IF = 2.942)
93. Silver cluster decorated graphene nanoflakes for selective and accurate detection of nitroaniline isomers; DFT calculations. Tabish Jadoon, Tariq Mahmood, **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2021**, 134, 106023 (IF = 4.644)
94. Regio- and stereoselective functionalization of alkenes with emphasis on mechanistic insight and sustainability concerns. Ghulam Bary, Muhammad Imran Jamil, Muhammad Arslan, Lubna Ghani, Waqar Ahmed, Haseen Ahmed, Gohar Zaman, **Khurshid Ayub**, Muhammad Sajid, Riaz Ahmad, Duohui Huang, Futi Liu, Yue Wang, *Journal of Saudi Chemical Society*, **2021**, 25, 101260 (IF = 4.644)
95. Zintl based superatom P_7M_2 (M=Li, Na, K & Be, Mg, Ca) clusters with excellent second and third-order nonlinear optical response, Atazaz Ahsin and **Khurshid Ayub***, *Materials Science in Semiconductor Processing*, **2021**, 134, 105986 (IF = 4.644)

96. Turning diamondoids into nonlinear optical materials by alkali metal substitution: A DFT investigation, Palwasha Khan, Tariq Mahmood, **Khurshid Ayub**, Sobia Tabassum, Mazhar Amjad Gilani, *Optics and Laser Technology*, **2021**, *142*, 107231 (IF = 4.939)
97. DFT study of super halogen doped borophene with enhanced nonlinear optical properties, Muhammad Ishaq; Rao Aqil Shehzad; Muhammad Yaseen, Saleem Iqbal, **Khurshid Ayub**; Javed Iqbal, *Journal of Molecular Modeling*, **2021**, *27*:188 (IF = 2.172)
98. Cu-doped phosphorene as highly efficient single atom catalyst for CO oxidation: A DFT study, Muhammad Hamid Butt, Syeda Huda Mehdi Zaidi, Nabeela, Aysha Khan, **Khurshid Ayub**, Muhammad Yar, Muhammad Ali Hashmi, Mirza Arfan Yawer, Muhammad Abid Zia, *Journal of Molecular Catalysis A: Chemical*, **2021**, *509*, 111630 (IF = 5.089)
99. Designing of Inorganic Al₁₂N₁₂ Nanocluster with Fe, Co, Ni, Cu, and Zn Metals for Efficient Hydrogen Storage Materials. Muhammad Yasir Mehboob, Fakhar Hussain, Riaz Hussain, Shaukat Ali, Zobia Irshad, **Khurshid Ayub** and Muhammad Adnan, *Journal of Computational Biophysics and Chemistry*, **2021**, *20*(4), 359-375 (IF = 0.0)
100. Inorganic electrides of alkali metal doped Zn₁₂O₁₂ nanocage with excellent nonlinear optical response, Saima Khan, Mazhar Amjad Gilani, Sajida Munsif, Shabbir Muhammad, Ralf Ludwig and **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2021**, *106*, 107935 (IF = 2.942)
101. Therapeutic potential of graphyne as a new drug-delivery system for daunorubicin to treat cancer: A DFT study, Iqra Munir, Mehvish Perveen, Sidra Nazir, Rasheed Ahmad Khera, Ali Raza Ayub, **Khurshid Ayub** and Javed Iqbal, *Journal of Molecular Liquids*, **2021**, *336*, 116327 (IF = 6.633)
102. Facile synthesis, DNA binding, urease inhibition, anti-oxidant, molecular docking and DFT studies of 3-(3-Bromo-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone and 3-(3-Bromo-5 chloro-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone, Faiz Rasool, Muhammad Khalid, Muahammad Yar, **Khurshid Ayub**, Muhammad Tariq, Ajaz Hussain,, Mehreen Lateef, Muhammad Kashif, Sana Iqbal, *Journal of Molecular Liquids*, **2021**, *336*, 116302 (IF = 6.633)
103. Theoretical and experimental investigation of CO₂ capture through choline chloride based supported deep eutectic liquid membranes, Manzar Ishaq, Mazhar Amjad Gilani, Faizan Ahmad, Zabila Muhammad Afzal, Ifra Arshad, Muhammad Roil Bilad, **Khurshid Ayub** and Asim Laeeq Khan, *Journal of Molecular Liquids*, **2021**, *336*, 116234, (IF= 6.633)
104. New strategy of bi-alkali metal doping to design boron phosphide nanocages of high nonlinear optical response with better thermodynamic stability. Rimsha Baloach, **Khurshid Ayub**, Tariq Mahmood, Anila Asif, Sobia Tabassum and Mazhar Amjad

Gilani, *Journal of Inorganic and Organometallic Polymers and Materials*, **2021**, 31, 3062-3076 (IF = 3.518)

- 105.** Oxacarbon superalkali $C_3X_3Y_3$ ($X = O, S$ and $Y = Li, Na, K$) clusters as excess electron compounds for remarkable static and dynamic NLO response, Atazaz Ahsin, **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2021**, 106, 107922 (IF = 2.942)
- 106.** Unprecedented saturation limit achieved by inorganic polycationic cluster $(Sb_7Te_8)5^+$ for light noble gases (He & Ne). Maryam Munir, Muhammad Yar, Faiza Ahsan, **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2021**, 106, 107910 (IF = 2.942)
- 107.** Influence of bi-alkali metals doping over $Al_{12}N_{12}$ nanocage on stability and optoelectronic properties: A DFT investigation, Muhammad Sohail, Faiqa Khaliq, Tariq Mahmood, **Khurshid Ayub**, Sobia Tabassum and Mazhar Amjad Gilani, *Radiation Chemistry and Physics*, **2021**, 184, 109457 (IF = 2.776)
- 108.** Study of nonlinear optical properties of superhalogen and superalkali doped phosphorene, Rida Khan, Rasheed Ahmad Khera, Asmat Ullah Khan, Ayesha Ayoub, Naseem Iqbal, **Khurshid Ayub**, Javed Iqbal, *Journal of Molecular Structure*, **2021**, 1236, 130348 (IF= 3.841)
- 109.** In Silico designing of $Mg_{12}O_{12}$ nanoclusters with late transition metal for NO_2 adsorption: An efficient approach towards development of NO_2 sensing materials, Shahid Hussain, Shahzad Ali Shahid Chatha, Abdullah Ijaz Hussain, Riaz Hussain, Muhammad Yasir Mehboob, Asim Mansha, Nabeel Shahzad, **Khurshid Ayub***, *ACS Omega*, **2021**, 6, 14191 (IF= 4.132)
- 110.** Quantum chemical study on sensing of NH_3 , NF_3 , NCl_3 and NBr_3 by using cyclic tetrapyrrole. Misbah Asif; Hasnain Sajid; Faizan Ullah; Sidra Khan; **Khurshid Ayub**; Mazhar Amjad Gilani; Muhammad Arshad; Mohammed Salim Akhter; Tariq Mahmood, *Computational and Theoretical Chemistry*, **2021**, 1199, 113221 (IF = 2.292)
- 111.** Electronic structure of polypyrrole composited with low percent of graphene nanofiller, Zulqarnain Chughtai, Muhammad Yar, Muhammad Ali Hashmi, **Khurshid Ayub***, *Physical Chemistry Chemical Physics*, **2021**, 23, 8557-8570 (IF= 3.945)
- 112.** Effective adsorption of A-series chemical warfare agents on graphdiyne nanoflake; A DFT study. Hasnain Sajid, Sidra Khan, **Khurshid Ayub** and Tariq Mahmood. *Journal of Molecular Modeling*. **2021**, 27:117 (IF = 2.172)
- 113.** DFT study on the sensitivity of silver-graphene quantum dots for vital and harmful analytes, Tabish Jadoon, Tariq Mahmood and **Khurshid Ayub***, *Journal of Physics and Chemistry of Solids*, **2021**, 153, 110028 (IF 4.383)
- 114.** Exploring Li_4N and Li_4O superalkalis as efficient dopants for $Al_{12}N_{12}$ nanocage to design high performance nonlinear optical materials with high thermodynamic stability, Faiqa Khalid, Tariq Mahmood, Khurshid Ayub, Sobia Tabassum, Mazhar Amjad Gilani, *Polyhedron*, **2021**, 200, 115145 (IF = 2.975)

115. Hydrogen adsorption on Ge_5^{2-} , Ge_9^{2-} and Sn_9^{2-} Zintl clusters: A DFT study. Hasnain Sajid, Sana Malik, Umer Rashid, Tariq Mahmood, **Khurshid Ayub***, *Computational and Theoretical Chemistry*, **2021**, 1199, 113191 (IF = 2.292)
116. Adsorption and sensor applications of C_2N surface for G-series and mustard series chemical warfare agents, Muhammad Yar, Faiza Ahsan, Adnan Gulzar and **Khurshid Ayub***, *Microporous and Mesoporous Materials*, **2021**, 317, 110984 (IF = 5.876)
117. DFT studies of Single and multiple alkali metals doped C_{24} fullerene for optical and optoelectronic applications. Naveen Kosar, Hira Tahir, **Khurshid Ayub** and Tariq Mahmood. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107867 (IF = 2.942)
118. The co-crystal of copper(II) phenanthroline chloride complex hydrate with p-aminobenzoic acid: structure, cytotoxicity, thermal analysis and DFT calculation, Hassan H. Hammud, Gregory J. McManus, Michael J. Zaworotko, Rola N. Tabesh, Hairul Islam M. Ibrahim, **Khurshid Ayub** and Ralf Ludwig, *Monatshefte für Chemie - Chemical Monthly*, **2021**, 152, 323-336 (IF = 1.613)
119. DFT study of superhalogen (AlF_4) doped boron nitride for tuning their nonlinear optical properties, Asmat Ullah Khan, Shabbir Muhammad, Rasheed Ahmad Khera, Rao Aqil Shahzad, **Khurshid Ayub** and Javed Iqbal, *Optik*, **2021**, 231, 166464 (IF=2.84)
120. DFT study of superhalogen and superalkali doped graphitic carbon nitride and its non-linear optical properties. Asmat Ullah Khan, Rasheed Ahmad Khera, Naveed Anjum, Rao Aqil Shahzad, Saleem Iqbal, **Khurshid Ayub*** and Javed Iqbal, *RSC Advances*, **2021**, 11, 7779-7789 (IF = 4.036)
121. Theoretical modification of C_{24} fullerene with single and multiple alkaline earth metal atoms for their potential use as NLO materials. Naveen Kosar, Hira Tahir, **Khurshid Ayub**, Mazhar Amjad Gilani and Tariq Mahmood. *Journal of Physics and Chemistry of Solids*. **2021**, 152, 109972 (IF = 4.383)
122. Remarkable static and dynamic NLO response of alkalis and superalkalis doped macrocyclic [hexa-]thiophene complexes; a DFT approach. Hasnain Sajid, Faizan Ullah, Sidra Khan, **Khurshid Ayub**, Muhammad Arshad and Tariq Mahmood. *RSC Advances*, **2021**, 11, 4118-4128 (IF = 4.036)
123. Storage and permeation of hydrogen molecule, atom and ions (H^+ and H^-) through silicon carbide nanotube; a DFT approach, Naveen Kosar, Sajida Munsif, **Khurshid Ayub** and Tariq Mahmood, *International Journal of Hydrogen energy*, **2021**, 46, 9163-9173 (IF = 7.139)
124. Endohedral metallofullerene electrides of $\text{Ca}_{12}\text{O}_{12}$ with remarkable nonlinear optical response, Annum Ahsan, Saima Khan, Mazhar Amjad Gilani and **Khurshid Ayub***, *RSC Advances*, **2021**, 11, 1569 -1580 (IF = 4.036)

125. Nonlinear optical response of first-row transition metal doped $\text{Al}_{12}\text{P}_{12}$ nanoclusters: A first principles study; Faizan Ullah, Sundus Irshad, Saima Khan, Muhammad Ali Hashmi, Ralf Ludwig, Tariq Mahmood and **Khurshid Ayub***, *Journal of Physics and Chemistry of Solids*, **2021**, *151*, 109914 (IF = 4.383)
126. Sensing of toxic Lewisite (L1, L2 & L3) molecules by graphdiyne nanoflake using DFT calculations and QTAIM analysis. Sidra Khan, Hasnain Sajid, **Khurshid Ayub** and Tariq Mahmood. *Journal of Physical Organic Chemistry*, **2021**, *34*, e4181 (IF = 2.155)
127. Silver cluster (Ag_6) decorated coronene as non-enzymatic sensor for glucose and H_2O_2 . Tabish Jadoon, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2021**, *103*, 107824 (IF = 2.942)
128. Theoretical investigation of superalkali clusters M_2OCN and M_2NCO (where $\text{M}=\text{Li, Na, K}$) as excess electron system with significant static and dynamic nonlinear optical response, Atazaz Ahsin, **Khurshid Ayub***, *Optik*, **2020**, *226*, 16603 (IF = 2.84)
129. Surface functionalization of twisted graphene $\text{C}_{32}\text{H}_{15}$ and $\text{C}_{104}\text{H}_{52}$ derivatives with alkalis and superalkalis for NLO response; a DFT study. Naveen Kosar, **Khurshid Ayub**, Tariq Mahmood, *Journal of Molecular Graphics and Modelling*, **2021**, *102*, 107794 (IF = 2.942)
130. Efficient Cu decorated inorganic $\text{B}_{12}\text{P}_{12}$ nanoclusters for sensing toxic COCl_2 gas: A detailed DFT study. Faiza Younas, Muhammad Yasir Mehboob, Khurshid Ayub, Riaz Hussain, Ali Umar, Muhammad Usman Khan, Zobia Irshad, Muhammad Adnan, *Journal of Computational Biophysics and Chemistry*, **2021**, *20*, 85-97 (IF = 0.0)
131. Enhanced linear and nonlinear optical response of superhalogen (Al_7) doped graphitic carbon nitride ($g\text{-C}_3\text{N}_4$), Rao Aqil Shehzad, Javed Iqbal, **Khurshid Ayub**, Faisal Nawaz, Shabbir Muhammad, Ali Raza Ayub, Saleem Iqbal, *Optik*, **2021**, *226*, 165923 (IF = 2.84)
132. Exploring the twisted molecular configurations for tuning their optical and nonlinear optical response properties; A quantum chemical approach. Shabbir Muhammad, Chin-Hung Lai, Abdullah G Al-Sehemi, Thamaa Alshahrani, Javed Iqbal, **Khurshid Ayub** and Mukesh Choudhary, *Journal of Molecular Graphics and Modelling* **2021**, *102*, 107766 (IF = 2.942)
133. Theoretical Investigation of halides encapsulated Na@B_{40} nanocage for potential applications as anodes for sodium ion batteries. Naveen Kosar, Faizan Ullah., **Khurshid Ayub**, Umer Rashid, Muhammad Imran, Muhammad Naeem Ahmed, *Materials Science in Semiconductor Processing*, **2021**, *121*, 105437 (IF = 4.644)

- 134.** First row transition metal decorated boron phosphide nanoclusters as nonlinear optical materials with high thermodynamic stability and enhanced electronic properties; A detailed quantum chemical study. Sundus Irshad, Faizan Ullah, Saima Khan, Ralf Ludwig, Tariq Mahmood and **Khurshid Ayub***, *Optics and Laser Technology*, **2021**, 134, 106570 (IF = 4.939)
- 135.** Designing of benzodithiophene core based small molecular acceptor for efficient non-fullerene organic solar cells, Muahmmad Yasir Mehboob, Muhammad Usman Khan, Riaz Hussain, Riaz Hussain, **Khurshid Ayub**, Abdul Sattar, Muhammad Kaleem Ahmad, Zobia Irshad, Saira, Muhammad Adnan, *Spectrochimica Acta A: Molecular and Biomolecular Spectroscopy*, **2021**, 244, 118873 (IF = 4.831)
- 136.** Isatin-derived non-fullerene acceptors for efficient organic solar cells, Irfan Yousaf, Rasheed Ahmad Khera, Javed Iqbal, Sehrish Gul, Sobia Jabeen, Abayn Ugsab abd **Khurshid Ayub**, *Materials Science in Semiconductor Processing*, **2021**, 121, 105345 (IF = 4.644)
- 137.** Density Functional Theory, molecular docking and in vivo muscle relaxant, sedative, and analgesic studies of Indanone derivatives isolated from *Heterophragma adenophyllum* Abdullah S. M. Aljohani, Tareq Abu-Izneid, Zafar Ali Shah, Umer Rashid, **Khurshid Ayub**, Abdur Rauf, Naveed Muhammad, Fahad A. Alhumaydhi, Maria Asghar, Mohammad S. Mubarak, Mohammad Ali Shariati Haiyuan Zhang *Journal of Biomolecular Structure and Dynamics*, **2021**, 39(17), 6488-6499 (IF = 5.235)
- 138.** Anticancer evaluation of a manganese complex on HeLa and MCF-7 cancer cells: design, deterministic solvothermal synthesis approach, Hirshfeld analysis, DNA binding, intracellular reactive oxygen species (ROS) production, electrochemical characterization and density functional theory, Saghir Abbas, Faisal Rashid, Emine Ulker, Sumera Zaib, **Khurshid Ayub**, Sana Ullah, Muhammad Arif Nadeem, Sammer Yousuf, Ralf Ludwig, Saqib Ali and Jamshed Iqbal, *Journal of Biomolecular Structure and Dynamics*. **2021**, 39(3), 1068-1081 (IF 5.235)

2020

- 139.** Polyaniline Emeraldine Salt as Selective Electrochemical Sensor for HBr over HCl: A Systematic Density Functional Theory Study through Oligomer Approach. Bilal Ahmed Farooqi, Ayesha Ashraf, Muhammad Yar, Ayesha Ashraf, Umar Farooq and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2020** 26, 332 (IF = 2.172)
- 140.** Selective detection and removal of picric acid by C2N surface from a mixture of nitro-explosives. Muhammad Yar, Ahmed Bilal, Muhammad Ali Hashmi, **Khurshid Ayub***, *New Journal of Chemistry*, **2020**, 44, 18646-18655 (IF = 3.927)

141. Synthesis, single-crystal X-ray diffraction, and in vitro biological evaluation of sodium, cobalt, and tin complexes of *o*-nitro-*o*-methoxyphenylacetic acid: experimental and theoretical investigation, Muhammad Danish, Muhammad Asam Raza, Sana Iftikhar, Muhammad Waseem Mumtaz, Muhammad Nawaz Tahir, Umer Rashid and **Khurshid Ayub**, *Monatshefte für Chemie - Chemical Monthly*, **2020**, *151*, 1727-1736 (IF = 1.613)
142. First-principles study for exploring the adsorption behavior of G-series nerve agents on graphdyine surface. Sidra Khan; Muhammad Yar; Naveen Kosar; **Khurshid Ayub**; Muhammad Arshad; Muhammad Nauman Zahid; Tariq Mahmood. *Computational and Theoretical Chemistry* **2020**, *1191*, 113043 (IF = 2.292)
143. Alkaline earth metals serving as source of excess electron for alkaline earth metals to impart large second and third order nonlinear optical response: A DFT Study. Atazaz Ahsin, Akhtar Ali and **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2020**, *101*,107759 (IF = 2.942)
144. Permeation of second row neutral elements through Al₁₂P₁₂ and B₁₂P₁₂ nanocages; A first principles study. Saira Sajjad, Muhammad Ali Hashmi, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2020**, *101*, 107748 (IF = 2.942)
145. Remarkable enhancement in sensor ability of polyaniline upon composite formation with ZnO for industrial effluents. Bilal Ahmed Farooqi, Muhammad Yar, Ayesha Ashraf, Umar Farooq, **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2020**, *101*, 107724 (IF = 2.942)
146. Graphene-polyaniline composite as superior electrochemical sensor for detection of cyano explosives. Bilal Ahmed Farooqi, Muhammad Yar, Ayesha Ashraf, Umar Farooq, **Khurshid Ayub***, *European Polymer Journal*, **2020**, *138*, 109981 (IF = 5.546)
147. Therapeutic potential of graphitic carbon nitride as a drug delivery system for cisplatin (anticancer drug): A DFT approach, Mehvish Perveen, Sidra Nazir, Ahmad Wahab Arshad, Muhammad Issa Khan, Maria Shamim, **Khurshid Ayub**, Muhammad Asif Khan, Javed Iqbal, *Biophysical Chemistry*, **2020**, *267*, 106461 (IF = 3.628)
148. Superhalogen doping: A new and effective approach to design materials with excellent static and dynamic NLO response, Hasnain Sajid, Faizan Ullah, Muhammad Yar, **Khurshid Ayub** and Tariq Mahmood, *New Journal of Chemistry*, **2020**, *44*,16358-16369 (IF = 3.927)
149. The C₂N surface as a highly selective sensor for the detection of nitrogen iodide from a mixture of NX₃ (X = Cl, Br, I) explosives. Muhammad Yar, Muhammad Ali Hashmi, **Khurshid Ayub***, *RSC Advances*, **2020**, *10*, 31997-32010 (IF = 4.036)

150. Exploration of adsorption behavior, electronic nature and NLO response of hydrogen adsorbed Alkali metals (Li, Na and K) encapsulated $Al_{12}N_{12}$ nanocages. Riaz Hussain, Muhammad Imran, Muhammad Ali, Muhammad Yasir Mehboob, Riaz Hussain, Muhammad Usman Khan, **Khurshid Ayub**, Mirza Arfan Yawer, Muhammad Saleem, Mohammed A. Assiri, Ahmad Irfan, *Journal of Theoretical and Computational Chemistry*, **2020**, 19, 08, 2050031 (IF = 0)
151. Comparative study on sensing abilities of polyaniline and graphene polyaniline composite sensors towards methylamine and ammonia, Bilal Ahmed Farooqi, Ayesha Ashraf, Umar Farooq and **Khurshid Ayub***, *Polymers for Advanced Technologies*, **2020**, 31, 3351-3360 (IF = 3.348)
152. Adsorption behaviour of chronic blistering agents on graphdiyne; excellent correlation among SAPT, reduced density gradient (RDG) and QTAIM analyses. Sidra Khan, Hasnain Sajid, **Khurshid Ayub** and Tariq Mahmood, *Journal of Molecular Liquids*, **2020**, 316, 113860 (IF = 6.633)
153. Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. Faiza Jilani. Javed Iqbal, Izza Shahid, Muahammad Yaseen, Muhammad Shabir Mahr, Muhammad Khalid, **Khurshid Ayub**, *Computational and Theoretical Chemistry*, **2020**, 1187, 112916 (IF = 2.292)
154. Janus alkaline earthides with excellent NLO response from sodium and potassium as source of excess electrons; a first principles study. Saira Sajjad, Akhtar Ali, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107668 (IF = 2.942)
155. Designing novel Zn decorated inorganic $B_{12}P_{12}$ nanoclusters with promising electronic properties. A step forward towards efficient CO_2 sensing materials. Shahid Hussain, Shahzad Ali Shahid Chatha, Abdullah Ijaz Hussain, Riaz Hussain, Muhammad Yasir Mehboob, Tahsin Gulzar, Asim Mansha, Nabeel Shahzad and **Khurshid Ayub***, *ACS Omega*, **2020**, 5(25), 15547-15556 (IF= 4.132)
156. Nonlinear optical response of sodium based superalkalis decorated graphdiyne surface; a DFT study. Naveen Kosar, Kiran Shahzadi, **Khurshid Ayub** and Tariq Mahmood, *Optik, International Journal of Light and Electron Optics*, **2020**, 218, 165033 (IF = 2.84)
157. Remarkable second and third order nonlinear optical properties of organometallic $C_6Li_6-M_3O$ electrides. Faizan Ullah, **Khurshid Ayub** and Tariq Mahmood, *New Journal of Chemistry*, **2020**, 44, 9822-9829 (IF = 3.927)

158. High sensitivity of graphdiyne surface toward detection of phosgene, thiophosgen and phosgenoxime; a first-principles study. Hasnain Sajid, Sidra Khan, **Khurshid Ayub** and Tariq Mahmood, *Journal of Molecular Graphics and Modelling*, **2020**, *100*, 107658 (IF = 2.942)
159. Density functional theory study of palladium clusters adsorption on graphene support Riaz Hussain, Muhammad Saeed, Muhammad Yasir Mehboob, Saif Ullah Khan, Muhammad Usman Khan, Muhammad Adnan, Mahmood Ahmed, Javed Iqbal and **Khurshid Ayub***, *RSC Advances* **2020**, *10*, 20595-50607 (IF = 4.036)
160. Carbon nitride 2-D surface as a highly selective electrochemical sensor for V-series nerve agents. Muhammad Yar, Muhammad Ali Hashmi, Ayesha Khan and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2020**, *311*, 113357 (IF = 6.633)
161. Adamanzane based alkaline earthides with excellent nonlinear optical response and ultraviolet transparency, Annum Ahsan and **Khurshid Ayub***, *Optics & Laser Technology*, **2020**, *129*, 106298 (IF = 4.939)
162. Enhancement in photovoltaic properties of *N,N*-diethylaniline based donor materials by bridging core modifications for efficient solar cells, Riaz Hussain, Muhammad Usman Khan, Muhammad Yasir Mehboob, Muhammad Khalid, Javed Iqbal, **Khurshid Ayub**, Muhammad Adnan, Mahmood Ahmed, Kainat Atiq and Khalid Mahmood, *ChemistrySelect*, **2020**, *5*, 1-14 (IF = 2.307)
163. Silver-graphene quantum dots based electrochemical sensor for trinitrotoluene and *p*-nitrophenol. Tabish Jadoon, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2020**, *306*, 112878 (IF = 6.633)
164. Outstanding NLO response of thermodynamically stable single and multiple alkaline earth metals doped C20 fullerene. Hira Tahir, Naveen Kosar, **Khurshid Ayub** and Tariq Mahmood, *Journal of Molecular Liquids*, **2020**, *305*, 112875 (IF = 6.633)
165. Adsorption of phosgene gas on pristine and copper decorated B₁₂N₁₂ Nanocages: A comparative DFT study. Shahid Hussain, Riaz Hussain, Muhammad Yasir Mehboob, Shahzad Ali Shahid Chattha, Abdullah Ijaz Hussain, Ali Umar, Muhammad Usman Khan, Mahmood Ahmad, Muhammad Adnan, **Khurshid Ayub***, *ACS Omega*, **2020**, *5*(13), 7641-7650 (IF = 4.132)
166. Expanding the horizons of covalent organic frameworks to electrochemical sensors; A case study of CTF-FUM, Muhammad Yar and **Khurshid Ayub***, *Microporous and Mesoporous Materials*, **2020**, *300*, 110146 (IF = 5.876)
167. Designing alkoxy-induced based high performance near infrared sensitive small molecule acceptors for organic solar cells Muhammad Ans, Mahalingavelar Paramasivam, **Khurshid Ayub***, Ralf Ludwig, Muhammad Zahid and Javed Iqbal, *Journal of Molecular Liquids*, **2020**, *305*, 112829 (IF = 6.633)
168. High selectivity of cyclic tetrapyrrole over tetrafulran and tetrathiophene toward toxic chemicals; A first-principles study. Hasnain Sajid, Sidra Khan, **Khurshid Ayub** and Tariq Mahmood, *Microporous and Mesoporous Materials*. **2020**, *299*, 110126 (IF = 5.876)

169. Theoretical study on novel superalkali doped graphdiyne complexes: unique approach for the enhancement of electronic and nonlinear optical response. Naveen Kosar, Kiran Shahzadi, **Khurshid Ayub** and Tariq Mahmood *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107573 (IF = 2.942)
170. Synergic effect of pore size engineering and applied electric field on the controlled permeation of alkali metal atoms and ions across pristine and defected h-BN sheet. Sajida Munsif, Naveen Kosar, Muhammad Ali Hashmi, Tariq Mahmood, Mazhar Amjad Gilani, **Khurshid Ayub***. *New Journal of Chemistry*, **2020**, 44, 7891-7901 (IF 3.927)
171. Cyclic versus straight chain oligofuran as sensor: A detailed DFT study. Hasnain Sajid, Faizan Ullah, **Khurshid Ayub** and Tariq Mahmood, *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107569 (IF 2.924)
172. Permeation selectivity of alkali metal ions through crown ether based ion channels. Arsalan Ahmed, Muhammad Ali Hashmi and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2020**, 302, 112577 (IF = 6.633)
173. Theoretical investigation on radical anion promoted electrocyclization in photochromes. Nadia Bibi, Naveen Kosar, **Khurshid Ayub**, Tariq Mahmood. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107550 (IF = 2.942)
174. Exceptional NLO response and deep ultraviolet transparency of superalkali doped macrocyclic oligofuran: A detailed DFT study. Hasnain Sajid, **Khurshid Ayub** and Tariq Mahmood. *New Journal of Chemistry*, **2020**, 44, 2609-2618 (IF = 3.927)
175. Zinc doped boron phosphide nanocluster as efficient sensor for SO₂. Shahid Hussain, Shahzad Ali Shahid Chatha, Abdullah Ijaz Hussain, Riaz Hussain, Muhammad Yasir Mehboob, Shabbir Muhammad, Zaheer Ahmad, **Khurshid ayub***, *Journal of Chemistry*, **2020**, 2629596, 1-12 (IF= 3.21)
176. Electronic structure of polythiophene gas sensors for chlorinated analytes. Ayesha Ashraf, Umar Farooq, Bilal Ahmed Farooqi and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2020**, 26:44 (IF = 2.172)
177. Alkaline earth metal decorated phosphide nanoclusters for potential applications as high performance NLO materials; A first principle study. Faizan Ullah, Naveen Kosar, Asgar Ali, Maria, Tariq Mahmood, **Khurshid Ayub***. *Physica E: Low Dimensional Systems and Nanostructures*. **2020**, 118, 113906 (IF= 3.369)
178. Significant nonlinear optical response of alkaline earth metals doped beryllium and magnesium oxide nanocages. Naveen Kosar, Saman Gul, **Khurshid Ayub**, Ali Bahader, Mazhar Amjad Gilani, Muhammad Arshad, Tariq Mahmood, *Materials Chemistry and Physics*, **2020**, 242, 122507 (IF = 4.778)

- 179.** Design of Novel inorganic alkaline earth metal doped aluminum nitride complexes (AEM@Al₁₂N₁₂) with high chemical stability, improved electronic properties and large nonlinear optical response. Faizan Ullah, Naveen Kosar, Asghar Ali, Maria, Tariq Mahmood and **Khurshid Ayub***, *Optik, International Journal of Light and Electron Optics*, **2020**, 207, 163792 (IF = 2.84)
- 180.** Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of C–Mg bond of Grignard reagent. Naveen Kosar, **Khurshid Ayub**, Mazhar Amjad Gilani, Faheem Shah and Tariq Mahmood, *International Journal of Quantum Chemistry*, **2020**, 120, e26106 (IF = 2.437)
- 181.** Tuning opto-electronic properties of alkoxy-induced based electron acceptors in infrared region for high performance organic solar cells. Muhammad Ans, **Khurshid Ayub***, Xiudi Xian, Javed Iqbal, *Journal of Molecular Liquids*, **2020**, 298, 111963 (IF = 6.633)
- 182.** Silver clusters tune up electronic properties of graphene nanoflakes: A comprehensive theoretical study, Tabish Jadoon, Kevin Carter-Fenk, Muhammad Bilal Ahmed Siddique, John Herbert, Riaz Hussain, Sarosh Iqbal, Javed Khattak, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2020**, 297, 111902 (IF = 6.633)
- 183.** Extremely large nonlinear optical response and excellent electronic stability of true alkaline earthides based on hexaammine complexant, Annum Ahsan and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2020**, 297, 111899 (IF = 6.633)
- 184.** Design of novel superalkali doped silicon carbide nanocages with giant nonlinear optical response. Faizan Ullah, Naveen Kosar, Mazhar Gilani, **Khurshid Ayub**, Muhammad Nadeem Arshad and Tariq Mahmood, *Optics and Laser Technology*, **2020**, 122, 105855 (IF= 4.939)
- 185.** Synthesis, crystal structures, computational studies and α -amylase inhibition of three novel 1,3,4-oxadiazole derivatives. Syeda Shamila Hamdani, Bilal Ahmad Khan, Muhammad Naeem Ahmed, Shahid Hameed, Kulsoom Akhter, **Khurshid Ayub** and Tariq Mahmood, *Journal of Molecular Structure*, **2020**, 1200, 127085 (IF = 3.841)
- 186.** Enhancement in the mechanical property of NBR/PVC nanocomposite by using sulfur and electron beam curing in the presence of Cloisite 30B nanoclay. Ali Shokuhi Rad, Elahe Aali, S Hallajian, Davood Zangeneh, Mitra Tavakoli, **Khurshid Ayub**. M. Peyravi, *Journal of Macromolecular Science PART A*, **2020**, 57, 123-132 (IF = 2.216)

- 187.** Interaction of graphene quantum dots with oligothiophene: A comprehensive theoretical study. Ayesha Ashraf, Kevin Carter-Fenk, John M Herbert, Bilal Ahmad Farooqi, Umar Farooq and **Khurshid Ayub***. *Journal of Physical Chemistry C*, **2019**, *123*, 29556-29570 (IF = **4.177**)
- 188.** Nitrogenated holey graphene (C₂N) surface as highly selective electrochemical sensor for ammonia, Muhamad Yar, Muhammad Ali Hashmi and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2019**, *296*, 111929 (IF = **6.633**)
- 189.** External stimulus controlled recombination of hydrogen in photochromic dithienylethene frustrated lewis pairs. Fazl-i-Sattar, Arsalan Ahmed, Habib Ullah, Zakir Ullah, Muhammad Tariq and **Khurshid Ayub***, *International Journal of Hydrogen Energy*, **2019**, *44*, 31141-31152 (IF = **7.139**)
- 190.** Designing dithienonaphthalene based acceptor materials with promising photovoltaic parameters for organic solar cells, Muhammad Ans, Javed Iqbal, Ijaz Ahmad Bhatti and **Khurshid Ayub***, *RSC Advances*, **2019**, *9*, 34496-34505 (IF = **4.036**)
- 191.** Exploring the potential of novel transition metal complexes derived from ONO donor type ligand: a quantum chemical study. Shamraiz Hussain Talib, Sajjad Hussain, Shabbir Muhammad, Baskaran Sambath, Javed Iqbal and **Khurshid Ayub**, *Journal of Molecular Modeling*, **2019**, *25*(9): 284 (IF = **2.172**)
- 192.** Doping superalkali on Zn₁₂O₁₂ nanocage constitutes a superior approach to fabricate stable and high-performance nonlinear optical materials, Naveen Kosar, Tariq Mahmood, **Khurshid Ayub**, Sobia Tabassum, Muhammad Arshad and Mazhar Amjad Gilani, *Optics and Laser Technology*, **2019**, *120*: 105753 (IF = **4.939**)
- 193.** A comprehensive DFT study on sensing abilities of cyclic oligothiophenes (nCT), Hasnain Sajid, **Khurshid Ayub** and Tariq Mahmood, *New Journal of Chemistry*, **2019**, *43*, 14120-14133 (IF = **3.925**)
- 194.** DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer, Amina Tariq, Sidra Nazir, Ahmad Wahab Arshad, Faisal Nawaz, **Khurshid Ayub***, Javed Iqbal, *RSC Advances*, **2019**, *9*, 24325-24332 (IF = **4.036**)
- 195.** Density functional theory, molecular docking and bioassay studies on (S)-2-hydroxy-N-(2S,3S,4R,E)-1,3,4 trihydroxyicos-16-en-2-yl)tricosanamide Taj Ur Rahman, Muhammad Aurang Zeb*, De-Bing Pu, Wajiha Liaqat, **Khurshid Ayub**, Wei-Lie Xiao, Tariq Mahmood, Muhammad Sajid, Riaz Hussain, *Heliyon*, **2019**, *5*, e02038 (IF = **3.776**)
- 196.** Designing dithienothiophene (DTT) based donor materials with efficient photovoltaic parameters for organic solar cells. Muhammad Ans, Farah Manzoor, **Khurshid Ayub**, Faisal Nawaz and Javed Iqbal. *Journal of Molecular Modeling*, **2019**, *25*: 222 (IF = **2.172**)

197. Density functional theory study of structural, electronic and CO adsorption properties of anionic Sc_n^- ($n = 2-13$) clusters. Saira Sajjad, Muhammad Ali Hashmi, Tariq Mahmood and **Khurshid Ayub***, *Computational and Theoretical Chemistry*, **2019**, *1163*, 112511 (IF = 2.292)
198. Highly selective acridinium based cyanine dyes for the detection of DNA base pairs (adenine, cytosine, guanine and thymine), Hasnain Sajid, **Khurshid Ayub**, Muhammad Arshad and Tariq Mahmood, *Computational and Theoretical Chemistry*, **2019**, *1163*, 112509 (IF = 2.292)
199. Theoretical study on design of novel superalkalis doped graphdiyne: a new donor-acceptor (D- π -A) strategy for enhancing NLO response. Kiran Shehzadi, **Khurshid Ayub** and Tariq Mahmood, *Applied Surface Science*, **2019**, *492*, 255-263 (IF = 7.392)
200. A combined experimental and computational study of 2,2'-(diazene-1,2-diylbis(4,1-phenylene))bis(6-(butylamino)-1H-benzo[de]isoquinoline-1,3(2H)-dione): Synthesis, optical and nonlinear optical properties. Santosh Kumar, Shabbir Muhammad, Joonseok Koh, Muhammad Khalid and **Khurshid Ayub**. *Optik, International Journal of Light and Electron Optics*, **2019**, *192*, 162952 (IF = 2.84)
201. Role of pyridine nitrogen in palladium catalyzed imine hydrolysis; A case study of (E)-1-(3-bromothiophen-2-yl)-N-(4-methylpyridin-2-yl)methanimine. Gulraiz Ahmad, Nasir Rasool, Komal Rizwan, Atif Ali Altaf, Tariq Mahmood, **Khurshid Ayub**, Umer Rashid, Mohd Zobir Hussein. *Molecules*, **2019**, *24*, 2609 (IF = 4.927)
202. Development of fullerene free acceptors molecules for organic solar cells: A step way forward toward efficient organic solar cells. Muhammad Ans, **Khurshid Ayub**, Shabbir Muhammad and Javed Iqbal, *Computational and Theoretical Chemistry*, **2019**, *1161*, 26-38. (IF = 2.292)
203. Change in the electronic and nonlinear optical properties of fullerene through its incorporation with Sc-, Fe-, Cu-, and Zn transition metals Ali Shokuhi Rad and **Khurshid Ayub**. *Applied Physics A*, **2019**, *125*:430 (IF = 2.983)
204. Thermal decomposition of *syn*- and *anti*-dihydroxyrenes; functional group dependent decomposition pathway. Bibi Saima, Yan Alexandar Wang, Riaz Hussain, Shabbir Muhammad and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2019**, *25*:215 (IF = 2.172)
205. Synthesis, structural properties, DFT studies, antimicrobial activities and DNA binding interactions of two newly synthesized organotin(IV) carboxylates Arshad Farooq Butt, Muhammad Naeem Ahmed, Moazzam Hussain Bhatti, Muhammad Aziz Choudhary, **Khurshid Ayub**, Muhammad Nawaz Tahir and Tariq Mahmood, *Journal of Molecular Structure*, **2019**, *1191*, 291-300 (IF = 3.841)
206. Superalkalis as a source of diffuse excess electrons in newly designed inorganic electrides with remarkable nonlinear response and deep ultraviolet transparency: A DFT study. Faizan Ullah, Naveen Kosar, **Khurshid Ayub**, Tariq Mahmood. *Applied Surface Science*. **2019**, *483*, 1118-1128 (IF = 7.392)

207. Dihydroazulene-vinylheptafulvene based photoswitchable Lewis pairs for tunable H₂ activation Nadeem S. Sheikh, Muhammad Ali Hashmi, Sajida Munsif, Mazhar Amjad Gilani, Mohammed A. Alkhalifah, Afsar Khan and **Khurshid Ayub***, *International Journal of Hydrogen Energy*, **2019**, 44, 14780-14795 (IF = 7.139)
208. Isolation, characterization and DFT study of epoxy ring containing withanolides from *Withania coagulans* Dunal. Shahid Ali Khan, Achyut Adhikari, **Khurshid Ayub**, Aliya Farooq, Saima Maher, Muhammad Nasimullah Qureshi, Abdur Rauf, Sher Bahadar Khan, Ralf Ludwig and Tariq Mahmood. *Spectrochimica Acta A: Molecular and Biomolecular Spectroscopy*, **2019**, 217, 113-121 (IF = 4.831)
209. Comparative investigation of sensor application of polypyrrole for gaseous analytes. Hasnain Sajid, Tariq Mahmood, Mian HR Mahmood and **Khurshid Ayub**. *Journal of Physical Organic Chemistry*. **2019**, e3960 (IF = 2.155)
210. Halides encapsulation in aluminum/boron phosphide nanoclusters: An effective strategy for high cell voltage in Na-ion battery. Naveen Kosar, Moneeba Asghar, **Khurshid Ayub***, Tariq Mahmood. *Materials Science in Semiconductor Processing*. **2019**, 97, 71-79 (IF = 4.644)
211. Theoretical study on a boron phosphide nanocage doped with superalkalis: novel electrides having significant nonlinear optical response. Faizan Ullah, Naveen Kosar, **Khurshid Ayub**, Mazhar Amjad Gilani and Tariq Mahmood, *New Journal of Chemistry*, **2019**, 43, 5727-5736 (IF = 3.925)
212. Designin of non-fullerene 3D star-shaped acceptors for organic solar cells. Muhammad Ans, Javed Iqbal, Bertil Eliasson, Muhammad Jawwad Saif, Hafiz Muhammad Asif, **Khurshid Ayub**, *Journal of Molecular Modeling*, **2019**, 25:129 (IF = 2.172)
213. Photo-tunable linear and nonlinear optical response of cyclophanediene-dihydropyrene photoswitches. Bibi Saima, Nasir Khan, Yasair S. S. Al-Faiyz, Ralf Ludwig, Wajid Rehman, Mian Habib-ur-Rehman, Nadeem S. Sheikh, **Khurshid Ayub***. *Journal of Molecular Graphics and Modelling*, **2019**, 88, 261-272 (IF = 2.942)
214. Spirobifluorene based small molecules as an alternative to traditional fullerene acceptors for organic solar cells. Muhammad Ans, Javed Iqbal, Ehsan Ali, Bertil Eliasson and **Khurshid Ayub**, *Materials Science in Semiconductor Processing*. **2019**, 94, 97-106 (IF = 4.644)
215. Benchmark DFT Studies on C-CN homolytic cleavage and screening the substitution effect on bond dissociation energy. Naveen Kosar, Mazhar Amjad Gilani, **Khurshid Ayub** and Tariq Mahmood. *Journal of Molecular Modeling*, **2019**, 25:47 (IF = 2.172)
216. Designing indacenodithiophene based non-fullerene acceptors with donor-acceptor combined bridge for organic solar cells. Muhammad Ans, **Khurshid Ayub** ,

Ijaz Ahmad Bhatti and Javed Iqbal, *RSC Advances*, **2019**, 9, 3605-3617 (IF =4.036)

217. Opto-electronic properties of non-fullerene fused-undecacyclic electron acceptors for organic solar cells. Muhammad Ans, Javed Iqbal, Bertil Eliasson, Muhammad Jawad Saif and **Khurshid Ayub**, *Computational Materials Science*, 2019, 159, 150-159 (IF = 3.572)
218. Synthesis and characterization of immobilized 1-(1,3-diphenyl-5-hydroxy-1H-pyrazol-4-yl)ethanone on silica gel and its use for aqueous heavy metal removal. Farah Suhail, Madeeha Batool, Muhammad Imran Din, Misbahul Ain Khan, **Khurshid Ayub**, Sobia Tabassum, Asma Tufail Shah, *Desalination and Water Treatment*, **2019**, 142, 213-224 (IF = 1.273)
219. Isolation, spectroscopic and density functional theory of two withanolide glycosides. Shahid Ali Khan, Saima Maher, Nadra Naheed, Maria, Tariq Mahmood, **Khurshid Ayub**, Aliya Farooq, Sher Bahadar Khan, Zarbad Shah, *Journal of Molecular Structure*, **2019**, 1177, 449-456 (IF = 3.841)
220. Antiradical, antimicrobial and enzyme inhibition evaluation of sulfonamide derived esters; synthesis, X-ray analysis and DFT studies. Muhammad Danish, Ayesha Bibi, Khola Gilani, Muhammad Asam Raza, Muhammad Ashfaq, Muhammd Nadeem Arshad, Abdullah Mohamed Asiri and **Khurshid Ayub**, *Journal of Molecular Structure*, **2019**, 1175, 379-388 (IF = 3.841)
221. Synthesis, X-ray crystal structure and spin polarized DFT study of high spin Mn based metal-organic framework. Saghir Abbas, **Khurshid Ayub**, Manzar Sohail, Saqib Ali, Ralf Ludwig, Muhammad Arif Nadeem, Shabbir Muhammad, *Journal of Molecular Structure*, **2019**, 1175, 439-444 (IF = 3.841)
222. Synthesis of novel metal complexes of 2-((phenyl (2-(4-sulfophenyl) hydrazono) methyl) diazenyl) benzoic acid formazan dyes: characterization, antimicrobial and optical properties studies on leather. Shakeel Ahmad Khan, Sammia Shahid, Sadia Kanwal, Komal Rizwan, Tariq Mahmood and **Khurshid Ayub**, *Journal of Molecular Structure*, **2019**, 1175, 73-89 (IF = 3.841)

2018

223. Designing three-dimensional (3D) non-fullerene small molecule acceptors with efficient photovoltaic parameters. Muhammad Ans, Javed Iqbal, Zahoor Ahmad, Shabbir Muhammad, Riaz Hussain, Bertil Eliasson and **Khurshid Ayub***, *ChemistrySelect*, **2018**, 3(45), 12797-12804 (IF = 2.307)
224. Detailed mechanistic study of radical mediated chemoselective phosphination of aryl halide Naveen Kosar, Tariq Mahmood, Farhan Hafeez, **Khurshid Ayub***, *ChemistrySelect* **2018**, 3(40), 11302-11308 (IF = 2.307)

225. Theoretical insight into structural and electronic properties of cationic Sc_n^+ ($n=2-13$): A benchmark study. Saira Sajjad, Tariq Mahmood, Ralf Ludwi and **Khurshid Ayub***. *Solid State Sciences*, **2018**, 86, 60-68 (IF = 3.752)
226. Sensor applications of polypyrrole for oxynitrogen analytes; A DFT study. Fatima Wasim, Naveen Kosar, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2018**, 24(11) :308 (IF = 2.172)
227. Designing dibenzosilole and methyl carbazole based donor materials with favourable photovoltaic parameters for bulk heterojunction organic solar cells. Zeenat Zara, Javed Iqbal, Sana Iftikhar, Salah Ud-Din Khan, Sajjad Haider, Bertil Eliasson and **Khurshid Ayub**, *Computational and Theoretical Chemistry*, **2018**, 1142, 45-56 (IF = 2.292)
228. Remarkable nonlinear optical response of alkali metal doped aluminum phosphide and boron phosphide nanoclusters, Sajida Munsif, Maria, Saima Khan, Asghar Ali, Mazhar Amjad Gilani, Javed Iqbal, Ralf Ludwig, **Khurshid Ayub***. *Journal of Molecular Liquids*, **2018**, 271, 51-64 (IF = 6.633)
229. Accurate theoretical method for homolytic cleavage of C-Sn bond: A benchmark approach, Naveen Kosar, **Khurshid Ayub***, Tariq Mahmood, *Computational and Theoretical Chemistry*, **2018**, 1140, 134-144 (IF = 2.292)
230. Facile synthesis of N-(4-bromophenyl)-1-(3-bromothiophen-2-yl)methanimine derivatives via Suzuki cross-coupling reaction: their characterization and DFT studies. Komal Rizwan, Nasir Rasool, Ravya Rehman, Tariq Mahmood, **Khurshid Ayub**, Tahir Rasheed, Gulraiz Ahmad, Ayesha Malik, Shakeel Ahmad Khan, Muhammad Nadeem Akhtar, Noorjahan Banu Alitheen and Muhammad Nazirul Mubin Aziz, *Chemistry Central Journal*, **2018**, 12:84 (IF = 4.095)
231. Receptor-spacer-fluorophore based coumarin-thiosemicarbazones as anion chemosensors with “turn on” response: spectroscopic and computational (DFT) studies. Muhammad Islam, Abdul Hameed, **Khurshid Ayub**, Muhamamd M. Naseer, Javid Hussain, Rima D. Alharthy, Asnuzilawati Asari, Ralf Ludwig, Mariya al-Rashida, Zahid Shafiq, *ChemistrySelect*, **2018**, 3, 7633-7642 (IF = 2.307)
232. Nonlinear optical, IR and orbital properties of Ni doped MgO nanoclusters: A DFT investigation, Ali Shokuhi Rad, **Khurshid Ayub***, *Computational and Theoretical Chemistry*, **2018**, 1138, 39-47 (IF = 2.292)
233. Novel acridine-based thiosemicarbazones as “Turn-on” chemosensors for selective recognition of fluoride anion: A spectroscopic and theoretical study, Ibanga Isaac, Iqra Munir, Mariya Al-Rashida, Syed Abid Ali, Zahid Shafiq, Muhammad Islam, Ralf Ludwig, **Khurshid Ayub***, Khalid Mohammad Khan, Abdul Hameed, *Royal Society Open Science*, **2018**, 5, 180646 (IF = 3.653)
234. Synthesis, characterisation, optical and nonlinear optical properties of thiazole and benzothiazole derivatives: a dual approach, Shabbir Muhammad, Santosh Kumar, Joonseok Koh, Munusamy Saravanabhavan, **Khurshid Ayub** & Mukesh Chaudhary, *Molecular Simulations*, **2018**, 44(15), 1191-1199 (IF = 2.346)

235. Synthesis, quantum chemical, in vitro acetyl cholinesterase inhibition and molecular docking studies of four new coumarin based pyrazolythiazole nuclei, Murtazaq Madni, Muhamad Naeem Ahmed, Shahid Hameed, Syed Wadood Ali Shah, Umer Rashid, **Khurshid Ayub**, Muhammad Nawaz Tahir and Tariq Mahmood, *Journal of Molecular Structure*, **2018**, 1168, 175-186 (IF = 3.841)
236. Density functional theory and surface reactivity study of bimetallic $Ag_n Y_m$ ($n+m = 10$) clusters, Riaz Hussain, Abdullah Ijaz Hussain, Shahzad Ali Shahid Chatha, Riaz Hussain, Usman Hanif and **Khurshid Ayub***, *Solid State Sciences*, **2018**, 80, 46-64 (IF = 3.752)
237. Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages, Yasir Arshad, Saima Khan, Muhammad Ali Hashmi and **Khurshid Ayub***, *New Journal of Chemistry*, **2018**, 42, 6976-6989 (IF = 3.925)
238. Palladium (0) catalyzed suzuki cross-coupling reaction of 2,5-dibromo-3-methylthiophene: selectivity, characterization, DFT studies and their biological evaluations Komal Rizwan, Muhammad Zubair, Nasir Rasool, Tariq Mahmood, **Khurshid Ayub**, Noorjahan Banu Alitheen, Muhammad Nadeem Akhtar, Faiz-ul-Hassan Nasim, Snober Mona Bukhary, Viqar Uddin Ahmad, Mubeen Rani, Muhammad Nazirul Mubin Aziz. *Chemistry Central Journal*, **2018**, 12:49 (IF = 4.095)
239. Synthesis, characterization, anti-leishmanial activity and *in silico* studies of 5-(4-methoxyphenyl)-2-(undecylthio)-1,3,4-oxadiazole, Muhammad Naeem Ahmed*, Iffat Ashraf, Khawaja Ansar Yasin, Sadiq ur Rehman, Rashid Mehmood, Umer Rashid, Tariq Mahmood, **Khurshid Ayub**, Muhammad Nawaz Tahir and Abdul Majeed Khan, *Journal of the Chemical Society of Pakistan*, **2018**, 40(5), 773-781 (IF = 0.698)
240. Diffusion of alkali metal atoms (Li, Na, K) on aluminum nitride and boron nitride nanocages; A density functional theory study, Sajida Munsif and **Khurshid Ayub***, *Journal of Molecular Liquids*, **2018**, 259, 249-259 (IF = 6.633)
241. Permeability and storage ability of inorganic $X_{12}Y_{12}$ fullerenes for lithium atom and ion, Sajida Munsif and **Khurshid Ayub**, *Chemical Physics Letters*, **2018**, 698, 51-59 (IF = 2.719)
242. How can nickel decoration affect H_2 adsorption on $B_{12}P_{12}$ nano heterostructures. Ali Shokuhi Rad, **Khurshid Ayub**, *Journal of Molecular Liquids*, **2018**, 255, 168-175 (IF = 6.633)
243. Theoretical calculations of the optical and electronic properties of dithienosilole and dithiophene based donor materials for organic solar cells. Farah Manzoor, Zeenat Zara, Javed Iqbal, Bertil Eliasson, Muhammad Shabir Mahr and **Khurshid Ayub**, *ChemistrySelect*, **2018**, 3(5) 1593-1601 (IF = 2.307)

244. Acridinedione as selective fluoride ion chemosensor: a detailed spectroscopic and quantum mechanical investigation. Nafees Iqbal, Syed Abid Ali, Iqra Munir, Saima Khan, **Khurshid Ayub**, Mariya al-Rashida, Muhammad Islam, Zahid Shafiq, Ralf Ludwig and Abdul Hameed. *RSC Advances*, **2018**, 8, 1993-2003 (IF= **4.306**)
245. High sensitivity of polypyrrole sensor for uric acid over urea, acetamide and sulfonamide: A density functional theory study, Hasnain Sajid, Tariq Mahmood and **Khurshid Ayub***, *Synthetic Metals*, **2018**, 235, 49-62 (IF = **4.0**)
246. Copper doped Al₁₂N₁₂ nano-cages: potential candidates for nonlinear optical materials, Urooj Gul, Mazhar Amjad Gilani, Sobia Tabassum, Tariq Mahmood, Abdulrahman I. Alharthi, MshariA. Alotaibi. Mohammed Geesi, Rizwan Sheikh, **Khurshid Ayub***, *Applied Physics A*, **2018**, 124: 14 (IF = **2.983**)
247. Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations, Saghir Abbas, Hafiza Huma Nasir, Sumera Zaib, Saqib Ali, Tariq Mahmood, **Khurshid Ayub**, Muhammad Nawaz Tahir, Jamshed Iqbal, *Journal of Molecular Structure*, **2018**, 1156, 193-200 (IF = **3.841**)
248. Selective arylation of phenol protected propyl bromide via Pd-catalysed Suzuki coupling reaction: synthesis, mechanistic studies by DFT calculations and their pharmacological aspects. Komal Rizwan, Sarosh Iqbal, Nasir Rasool, Muhammad Nadeem Akhtar, Muhammad Tayyab Ansari, Hira Farooq, Hira Israr, Tahir Rasheed, Seema Zareen, Tariq Mahmood, **Khurshid Ayub**, *Acta Poloniae Pharmaceutica - Drug Research*, **2018**, 75, 911-919 (IF = **0.555**)
249. Synthesis, crystal structures, computational studies and antimicrobial activity of new designed bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes, Muhammad Naeem Ahmed, Beenish Sadiq, Najim A. Al-Masoudi, Khawaja Ansar Yasin, Shahid Hameed, Tariq Mahmood, **Khurshid Ayub**, Muhammad Nawaz Tahir. *Journal of Molecular Structure*, **2018**, 1155, 403-413 (IF = **3.841**)
250. Nonlinear optical and electronic properties of Cr-, Ni-, and Ti- substituted C₂₀ fullerenes: A quantum-chemical study. Ali Shokuhi Rad, **Khurshid Ayub***, *Materials Research Bulletin*, **2018**, 97, 399-404 (IF = **5.6**)
251. Carbon-cobalt nanostructure as an efficient adsorbent of Malachite Green, Hassan H. Hammud, Bassem El Hamaoui, Nada H. Noubani, Xingliang Feng, Zhong-Shuai Wu, Klaus Müllen, and **Khurshid Ayub**, *Nanoscience & Nanotechnology-Asia*, **2018**, 8, 263-280

252. Substitutional doping of zirconium-, molybdenum-, ruthenium-, and palladium: An effective method to improve nonlinear optical and electronic properties of C₂₀ fullerene, Ali Shokuhi Rad, **Khurshid Ayub**, *Computational and Theoretical Chemistry*, **2017**, 1121, 68-75 (IF = 2.292)
253. An accurate comparative theoretical study of interaction of furan, pyrrole and thiophene with various gaseous analytes, Hasnain Sajid, Tariq Mahmood, **Khurshid Ayub***, *Journal of Molecular Modeling*, **2017**, 23, 295 (IF = 2.172)
254. Binding affinity and permeation ability of X₁₂Y₁₂ nanoclusters for helium and neon. **Khurshid Ayub***, *Journal of Molecular Liquids*, **2017**, 244, 124-134 (IF = 6.633)
255. Supported protic ionic liquid membrane based on 3-(trimethoxysilyl)propan-1-aminium acetate for the highly selective separation of CO₂, Asim Laeeq Khan, Ayesha Ilyas, Mazhar Amjad Gilani, I.F.J Vankelecom, nawshad Muhammad, **Khurshid Ayub**, *Journal of Membrane Science*, **2017**, 543, 301.-309 (IF = 10.53)
256. Role of dispersion corrected hybrid gga class in accurately calculating the bond dissociation energy of carbon halogen bond: a benchmark study, Naveen Kosar, Tariq Mahmood, **Khurshid Ayub***, *Journal of Molecular Structure*, **2017**, 1150, 447-458 (IF = 3.841)
257. A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. Zeenat Zara, Javed Iqbal, **Khurshid Ayub***, Muhammad Irfan, Ather Mahmood, Rasheed Ahmad Khera and Bertil Eliasson, *Journal of Molecular Structure*, **2017**, 1149, 282-298 (IF = 3.841)
258. Thiobiuret based Ni(II) and Co(III) complexes: synthesis, molecular structures and DFT studies, Saira Sherzaman, Sadiq-ur-Rehman, Muhammad Naeem Ahmed, Bilal Ahmed Khan, Tariq Mahmood, **Khurshid Ayub**, Muhammad Nawaz Tahir, *Journal of Molecular Structure*, **2017**, 1148, 15, 388-396 (IF = 3.841)
259. Estimation of optical rotation of γ -alkylidenebutenolide, cyclopropylamine, cyclopropyl-methanol and cyclopropanone based compounds by density functional theory (DFT) approach. Iram Shahzadi, Aqsa Shaukat, Zeenat Zara, Muhammad Irfan, Bertil Eliasson, **Khurshid Ayub**, Javed Iqbal, *Chirality*, **2017**, 29, 634-647 (IF = 2.183)
260. Crystal structure, spectroscopic, electronic, luminescent and nonlinear optical properties of (s)-4-Amino-5-(1-hydroxy-ethyl)-2,4-dihydro-[1,2,4]triazole-3-thione: A combined experimental and DFT study. Muhammad Nadeem, Uzma Yunus, Moazzam H. Bhatti, **Khurshid Ayub**, Mazhar Mehmood, Muhammad Jawwad Saif. *Journal of Physics and Chemistry of Solids*. **2017**, 110, 218-226 (IF = 4.383)

261. Mechanism of $Zn(OTf)_2$ catalyzed hydroamination-hydrogenation of alkynes with amines: Insight from theory. Riffat Un Nisa and **Khurshid Ayub***, *New Journal of Chemistry*, **2017**, *41*, 5082-5090 (IF = 3.925)
262. O_3 and SO_2 sensing concept on extended surface of $B_{12}N_{12}$ nanocages modified by Nickel decoration: A comprehensive DFT study. Ali Shokuhi Rad, **Khurshid Ayub**, *Solid State Sciences*, **2017**, *69*, 22-30 (IF = 3.752)
263. DFT study of acceleration of electrocyclization in photochromes under radical cationic conditions: Comparison with recent experimental data. Tariq Mahmood, Naveen Kosar and **Khurshid Ayub***, *Tetrahedron*, **2017**, *73*, 3521-3528 (IF = 2.388)
264. Adsorption of thiophene on the surfaces of $X_{12}Y_{12}$ ($X = Al, B$ and $Y = N, P$) nanoclusters; A DFT study, Ali Shokuhi Rad, **Khurshid Ayub***, *Journal of Molecular Liquids*, **2017**, *238*, 303-309 (IF = 6.633)
265. Synthesis and structural properties of N-(2-bromo-4-nitrophenyl)-3-methoxy-4-oxo-3,4-dihydro-2H-benzo[e][1,2]thiazine-3-carboxamide 1,1-dioxide: A comparative experimental and quantum chemical study. Muhammad Nadeem Arshad, Naveen Kosar, Abdullah M. Asiri, **Khurshid Ayub**, Islam Ullah Khan, Tariq Mahmood, *Journal of the Chemical Society of Pakistan*, **2017**, *39*, 5, 727-736 (IF = 0.698)
266. Benchmark study of bond dissociation energy of Si-X ($X = F, Cl, Br, N, O, H$ And C) bond using density functional theory (DFT), Sahar, Alina Bari, Zeenat Zara, Muhammad Irfan, Bertil Eliasson, **Khurshid Ayub***, Javed Iqbal, *Journal of Molecular Structure*, **2017**, *1143*, 8-19 (IF = 3.841)
267. Benchmark study of structural and vibrational properties of scandium clusters. Saira Sajjad, Maria, Tariq Mahmood, **Khurshid Ayub***, *Journal of Molecular Structure*, **2017**, *1142*, 139-147 (IF = 3.841)
268. Synthesis of functionalised fluorinated pyridine derivatives by site-selective Suzuki-Miyaura cross-coupling reactions of halogenated pyridines Muhammad Sharif, Khurram Shoaib, Shahzad Ahmed, Sebastian Reimann, Jamshed Iqbal, Muhammad Ali Hashmi, **Khurshid Ayub**, Nazym Yelibayeva, Meirambek Ospanov, Mirgul Zh. Turmukhanova, Zharylkasyn A. Abilov, Peter Langer, *Zeitschrift für Naturforschung B*, **2017**, *72*, 4, 263-279 (IF = 1.115)
269. Adsorption properties of acetylene and ethylene molecules onto pristine and nickel-decorated $Al_{12}N_{12}$ nanoclusters, Ali Shokuhi Rad and **Khurshid Ayub***, *Materials Chemistry and Physics*, **2017**, *194*, 337-344, (IF = 4.778)
270. Phosphides or nitrides for better NLO properties? a detailed comparative study of alkali metal doped nano-cages, Maria, Javed Iqbal, Ralf Ludwig and **Khurshid Ayub***, *Materials Research Bulletin*, **2017**, *92*, 113-122 (IF = 5.6)

271. Transportation of hydrogen atom and molecule through $X_{12}Y_{12}$ nano-cages, **Khurshid Ayub***, *International Journal of Hydrogen Energy*, **2017**, *42*, 16, 11439-11451 (IF = 7.139)
272. Synthesis, crystal structure, spectral analysis, DFT studies and antimicrobial activity of ethyl 6-(4-(ethoxycarbonyl)-1h-1,2,3-triazol-1-yl)pyridine-3-carboxylate, Muhammad Naeem Ahmed, Khawaja Ansar Yasin, Raja Ansar Hussain Khan, Tariq Mahmood, **Khurshid Ayub**, Dilshad Malik, Muhammad Hafeez, Abdul Majeed Khan and M. Nawaz Tahir, *Journal of the Chemical Society of Pakistan*, **2017**, *39(4)*, 640-649 (IF = 0.698)
273. Designing of Donor-Acceptor-Donor (D-A-D) type small molecule donor materials with photovoltaic parameters. Muhammad Irfan, Javed Iqbal, Sana Sadaf, Bertill Eliasson, Usman Ali Rana, Salah Ud Din Khan, **Khurshid Ayub***. *International Journal of Quantum Chemistry*, **2017**, *117*, 10, e25363 (IF = 2.437)
274. Density functional theory study of geometric and electronic properties of full range of bimetallic Ag_nY_m ($n + m = 10$) clusters. Riaz Hussain, Abdullah Ijaz Hussain, Shahzad Ali Shahid Chatha, Asim Mansha, **Khurshid Ayub***, *Journal of Alloys And Compounds*, **2017**, *705*, 232-246 (IF = 6.371)
275. DFT study of boron trichloride adsorption on the surface of $Al_{12}N_{12}$ nanocluster. Ali Shokuhi Rad, **Khurshid Ayub**, *Molecular Physics*. **2017**, *115*, 7, 879-884 (IF = 1.937)
276. Efficient synthesis of novel pyridine based derivatives via suzuki cross-coupling reaction of commercially available 5-bromo-2-methylpyridin-3-amine; quantum mechanical investigations and biological activities. Gulraiz Ahmad, Nasir Rasool *, Hafiz Mansoor Ikram, Sumreen Gul Khan, Tariq Mahmood, **Khurshid Ayub**, Muhammad Zubair, Eman Al-Zahrani, Usman Ali Rana, Muhammad Nadeem Akhtar, Noorjahan Banu Alitheen, *Molecules*, **2017**, *22(2)* 190 (IF = 4.927)
277. Synthesis, molecular structure, quantum mechanical studies and urease inhibition assay of two new isatin derived sulfonylhydrazides. Muhammad Arshad, Mehwish Jadoon, Zafar Iqbal, Mehwish Fatima, Muhammad Ali, **Khurshid Ayub**, Ashfaq Mahmood Qureshi, Muhammad Ashraf, Muhammad Nadeem Arshad, Abdullah M. Asiri, Amir Waseem, Tariq Mahmood, *Journal of Molecular Structure*, **2017**, *1133*, 80-89 (IF = 3.841)
278. Benchmark study of UV/Visible spectra of coumarin derivatives by computational approach. Muhammad Irfan, Javed Iqbal*, Bertil Eliason, **Khurshid Ayub***, Usman Ali Rana, Salah Ud Din Khan, *Journal of Molecular Structure*, **2017**, *1130*, 603-616 (IF = 3.841)
279. Fine tuning the optoelectronic properties of triphenylamine based donor molecules for organic solar cells Muhammad Adnan, Javed Iqbal, Shamsa Alina, Riaz Hussain, Muhammad Nadeem Akhtar, Muhammad Abid Rashid, Bertil Eliasson, **Khurshid Ayub***. *Zeitschrift für Physikalische Chemie*, **2017**, *231(6)*, 1127-1138 (IF = 4.315)

280. Synthesis, structural studies and biological activities of three new 2-(Pentadecylthio)-5-aryl-1,3,4-oxadiazoles. Muhammad Naeem Ahmed, Khawaja Ansar Yasin, Shahid Hameed, **Khurshid Ayub**, Ihsan ul Haq, M. Nawaz Tahir and Tariq Mahmood, *Journal of Molecular Structure*, **2017**, *1129*, 50-59 (IF = 3.841)

2016

281. Are phosphide nano-cages better than nitride nano-cages? A kinetic, thermodynamic and non-linear optical properties study of alkali metal encapsulated $X_{12}Y_{12}$ nano-cages, **Khurshid Ayub**, *Journal of Materials Chemistry C*, **2016**, *4*, 10919-10934 (IF = 8.067)
282. Theoretical study on non linear optical properties of alkali metal (Li, Na, K) doped aluminum nitride nano-cages, Maria, Javed Iqbal, **Khurshid Ayub***. *RSC Advances*, **2016**, *6*, 94228-94235 (IF = 4.036)
283. Synthesis, biological screening and molecular docking studies of some tin (IV) Schiff base adducts. Wajid Rehman, Rehana Yasmeen, Fazl Rahim, Muhammad Waseem, Cun-Yue Guo, Zonera Hassan, Umer Rashid and **Khurshid Ayub**, *Journal of Photochemistry and Photobiology B: Biology*. **2016**, *164*, 65-72. (IF = 6.814)
284. Density functional theory study of linear and non-linear optical properties of Dihydroazulene-Vinylheptafulvene photoswitches. Riffat Un Nisa, Nasir Shahzad and **Khurshid Ayub***, *Computational and Theoretical Chemistry*. **2016**, *1095*, 1-8 (IF = 2.292)
285. Coordination of nickel atoms with $Al_{12}X_{12}$ (X=N, P) nanocages enhances H_2 adsorption: A surface study by DFT. Ali Shokuhi Rad and **Khurshid Ayub***, *Vacuum*, **2016**, *133*, 70-80 (IF = 4.11)
286. Enhancement in hydrogen molecule adsorption on $B_{12}N_{12}$ nano-cluster by decoration of nickel, Ali Shokuhi Rad, **Khurshid Ayub**. *International Journal of Hydrogen Energy*, **2016**, *41*, 47, 22182-22191 (IF = 7.139)
287. Novel quinoxaline based chemosensors with selective dual mode of action: nucleophilic addition and host-guest type complex formation. Marium Ishtiaq, Iqra Munir, Mariya al-Rashida, Maria, **Khurshid Ayub**, Jamshed Iqbal, Ralf Ludwig, Khalid Mohammed Khan, Syed Abid Ali, and Abdul Hameed. *RSC Advances*, **2016**, *6*, 64009-64018 (IF = 4.036)
288. Adsorption of pyrrole on $Al_{12}N_{12}$, $Al_{12}P_{12}$, $B_{12}N_{12}$, and $B_{12}P_{12}$ fullerene-like nano-cages; a first principles study. Ali Shokuhi Rad, **Khurshid Ayub**, *Vacuum*, **2016**, *131*, 135-141 (IF = 4.11)
289. An accurate cost effective DFT approach to study sensor behaviour of polypyrrole for nitrate ion in gas and aqueous phase, Fatima Wasim, Tariq Mahmood and **Khurshid Ayub***. *Physical Chemistry Chemical Physics (PCCP)*, **2016**, *18*, 19236-19247 (IF = 3.945)

290. Synthesis, *in vitro* potential and computational studies on 2-amino-1,4-dihydropyrimidines as multitarget antibacterial ligands Muhammad Jawad Ahmad , Syed Fahad Hassan , Riffat Un Nisa , **Khurshid Ayub**, Muhammad Shahid Nadeem, Samina Nazir , Farzana Latif Ansari, Naveeda Akhter Qureshi and Umer Rashid, *Medicinal Chemistry Research*, **2016**, 25, 1877-1894 (IF = 2.351)
291. Enhanced electronic and non-linear optical properties of alkali metal (Li, Na, K) doped boron nitride nano-cages. Maria, Javed Iqbal and **Khurshid Ayub***, *Journal of Alloys and Compounds* **2016**, 687, 976-983 (IF = 6.371)
292. Detailed surface study of adsorbed nickel on Al₁₂N₁₂ nano-cage, Ali Shokuhi Rad, **Khurshid Ayub**, *Thin Solid Films*, **2016**, 612, 179-185 (IF = 2.358)
293. One Pot Selective Arylation of 2-Bromo-5-Chloro thiophene; Molecular Structure investigation via Density Functional Theory (DFT), X-ray Analysis and their Biological Activities. Nasir Rasool, Aqsa Kanwal, Tehmina Rasheed, Quratul Ain, **Khurshid Ayub**, Tariq Mahmood, Muhammad Zubair, Khalid Mohammad Khan, Muhammad Nadeem Arshad, Abdullah M. Asiri, Muhammad Zia-ul-haq, Hawa Z.E. Jaafar *. *International Journal of Molecular Sciences*, **2016**, 17(7), 912 (IF = 6.208)
294. Synthesis, spectral characterization and fluorescent assessment of 1,3,5-triaryl-2-pyrazoline derivatives: experimental and theoretical studies. Mohammad M Ibrahim, Mahmoud Al-Refai, **Khurshid Ayub** and Basem F Ali. *Journal of Fluorescence*, **2016**, 26, 1447-1455 (IF = 2.525)
295. Ni adsorption on Al₁₂P₁₂ nano-cage: A DFT study, Ali Shokuhi Rad, **Khurshid Ayub***, *Journal of Alloys and Compounds*, **2016**, 678, 317-324 (IF = 6.371)
296. Theoretical mechanistic investigation of Zinc(II) catalyzed oxidative amidation of benzyl alcohols with amines. Riffat Un Nisa, Zanib Sugheer, Muhammad Ali Hashmi, Muhammad Sharif, Mazhar Amjad Gilani, Ralf Ludwig, Tariq Mahmood, Javed Iqbal and **Khurshid Ayub***, *Polyhedron*, **2016**, 112, 34-42 (IF = 2.975)
297. Theoretical mechanistic investigation of zinc(ii) catalyzed oxidation of alcohols to aldehydes and esters. Riffat Un Nisa, Tariq Mahmood, Ralf Ludwig and **Khurshid Ayub***, *RSC Advances*, **2016**, 6, 31876-31883 (IF = 4.036)
298. Theoretical insight of thermal cyclophanediene to dihydropyrene electrocyclic reaction; a comparative study of Woodward-Hoffmann allowed and forbidden reactions. Bibi Saima, Afsar Khan, Riffat Un Nisa, Tariq Mahmood and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2016**, 22:81 (IF = 2.172)
299. Gas Hydrates Model for mechanistic investigation of Wittig reaction “on Water” **Khurshid Ayub***, Ralf Ludwig, *RSC Advances*, **2016**, 6, 23448-23458 (IF = 4.036)
300. A comparative density functional theory study of guanine chemisorption on Al₁₂N₁₂, Al₁₂P₁₂, B₁₂N₁₂ and B₁₂P₁₂ nano-cages. Ali Shokuhi Rad, **Khurshid Ayub**, *Journal of Alloys and Compounds*. **2016**, 672, 5, 161-169 (IF= 6.371)

- 301.** Quantum mechanical investigation on acceleration of electrocyclic reactions through transition metal catalysis. Riffat Un Nisa, Muhammad Ali Hashmi, Saira Sajjad, Tariq Mahmood, Javed Iqbal, **Khurshid Ayub***, *Journal of Organometallic Chemistry* **2016**, *808*, 78-86 (IF = **2.345**)
- 302.** One-pot synthesis of tetrazole-1,2,5,6-tetrahydronicotinonitriles and cholinesterase inhibition: probing the plausible reaction mechanism *via* computational studies, Abdul Hameed, Syeda Tazeen Zehra, Saba Abbas, Riffat Un Nisa, Tariq Mahmood, **Khurshid Ayub**, Mariya Al-Rashida, Jorgen Bajorath, Khalid Mohammed Khan and Jamshed Iqbal. *Bioorganic Chemistry*, **2016**, *65*, 38-47 (IF = **5.307**)
- 303.** Click one pot synthesis, spectral analysis, crystal structures, DFT studies and Brine shrimp cytotoxicity assay of two newly synthesized 1,4,5-trisubstituted 1,2,3-triazoles. Muhammad Naeem Ahmed, Khawaja Ansar Yasin, **Khurshid Ayub**, Tariq Mahmood, M. Nawaz Tahir, Bilal Ahmad Khan, Muhammad Hafeez, Madiha Ahmed, Ihsan-ul-Haq, *Journal of Molecular Structure*, **2016**, *1106*, 430-439 (IF = **3.841**)

2015

- 304.** Dyotropic rearrangement of bridgehead substituents in closed dithienylethenes: Conjugated versus non-conjugated analogues. Tariq Mahmood, Muhammad Arshad, Mazhar Amjad Gilani, Zafar Iqbal and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2015**, *21*, 321 (IF = **2.172**)
- 305.** Mechanistic insight of TiCl₄ catalyzed [3+3] cyclization of 1,3 -bis(silyl enol ethers) with 1,3-dielectrophiles, Riffat Un Nisa, Maria, Fatima Waseem, Tariq Mahmood, Ralf Ludwig, **Khurshid Ayub,*** *RSC Advances*, **2015**, *5*, 94304-94314 (IF = **4.036**)
- 306.** Synthesis, Density Functional Theory (DFT), urease inhibition and antimicrobial activities of 5-aryl thiophenes bearing sulphonylacetamide moiety, Mnaza Noreen , Nasir Rasool, Yasmeen Gull, Muhammad Zubair, Tariq Mahmood , **Khurshid Ayub**, Faiz-ul-Hassan Nasim, Asma Yaqoob, Muhammad Zia-Ul-Haq, Vincenzo De Feo. *Molecules*, **2015**, *20*, 19914-19928 (IF = **4.927**)
- 307.** Synthesis, structure, spectroscopic and DFT studies of zinc (II) and manganese (II) of 2-pyridine carboxaldehyde-N-methyl-N-2-pyridyl hydrazine. Basem F. Ali, Zaher Judeh and **Khurshid Ayub**, *Polyhedron*, **2015**, *101*, 118-125 (IF = **2.975**)
- 308.** Stereochemical effect of covalent chemistry on the electronic structure and properties of the carbon allotropes and graphene surfaces. Elena B. Bekyarova, Sandip Niyogi, Santanu Sarkar, Xiaojuan Tian, Mingguang Chen, Matthew L Moser, **Khurshid Ayub**, Reginald H. Mitchell and Robert C. Haddon. *Synthetic Metals*, **2015**, *210*, 80-84. (IF = **4.0**)

309. Combined experimental and theoretical study of poly(aniline-co-pyrrole) oligomer. Habib Ullah, Muhammad Kamran, Anwar-ul-Haq Ali Shah, Salma Bilal, Asif Ali Tahir and **Khurshid Ayub**. *Polymer*, **2015**, 72, 30-39 (IF = 4.432)
310. Synthesis, characterization of flavone, isoflavone, and 2,3-dihydrobenzofuran-3-carboxylate and density functional theory studies. Huma Aslam Bhatti, Nizam Uddin, **Khurshid Ayub**, Bibi Saima, Maliha Uroos, Jamshed Iqbal, Shazia Anjum, Mark Edward Light, Abdul Hameed and Khalid Mohammed Khan. *European Journal of Chemistry*, **2015**, 6(3), 305-313
311. Molecular and electronic structure elucidation of polypyrrole gas sensors. Salma Bibi, Habib Ullah, Shah Masood Ahmad, Anwar-ul-Haq Ali Shah, Salma Bilal, Asif Ali Tahir and **Khurshid Ayub**, *Journal of Physical Chemistry C*. **2015**, 119(28), 15994-16003, (IF = 4.177)
312. Towards thermally stable cyclophanediene-dihydropyrene photoswitches. Nasir Khan, Nadeem S. Sheikh, Ather Farooq Khan, Ralf Ludwig, Tariq Mahmood, Wajid Rehman, Yasair S. S. Al-Faiyz and **Khurshid Ayub***, *Journal of Molecular Modeling*, **2015**, 21:148 (IF = 2.172)
313. Density functional theory and phytochemical study of 8- hydroxyisodiospyrin. Zakir Ullah , Ata-ur-Rahman, Fazl-i-Sattar, Abdur Rauf , Muhammad Yaseen, W. Hassan, Muhammad Tariq, **Khurshid Ayub***, Asif Ali Tahir , Habib Ullah. *Journal of Molecular Structure*, **2015**, 1095, 69-78 (IF = 3.841)
314. Spectral and electronic properties of p-conjugated oligomers and polymers of Poly (o-chloroaniline-co-o-toluidine) calculated with density functional theory Shah Masood Ahmad, Salma Bibi, Salma Bilal, Anwar-ul-Haq Ali Shah, **Khurshid Ayub**. *Synthetic Metals*, **2015**, 205, 153-163. (IF = 4.0)
315. Spectroscopic and density functional theory studies of 7-hydroxy-3'-methoxyisoflavone: a new isoflavone from the seeds of indigofera heterantha (Wall).Taj Ur Rahman, Ghias Uddin, Riffat Un Nisa, Ralf Ludwig, Wajiha Liaqat Tariq Mahmood, Ghulam Mohammad, M. Iqbal Choudhary and **Khurshid Ayub***. *Spectrochimica Acta Part A: Molecular and Biomolecular spectroscopy*, **2015**. 148, 375-381 (IF = 4.831)
316. Aromaticity of 15,16-dimethyldihydropyrene relative to benzene and strain energies of elusive [e]-fused bis-dimethyldihydropyrenes. **Khurshid Ayub***, *Computational and Theoretical Chemistry*, **2015**, 1063, 42-49 (IF = 2.292)
317. Synthesis, crystal structures and spectroscopic properties of triazine based hydrazone derivatives; a comparative experimental-theoretical Study. Muhammad Nadeem Arshad, Aisha Bibi, Tariq Mahmood, Abdullah M. Asiri. **Khurshid Ayub**, *Molecules*, **2015**. 20, 5851-5874 (IF = 4.927)
318. Aromaticities of five membered heterocycles through dimethyldihydropyrenes probe by magnetic and geometric criteria. Maria, **Khurshid Ayub***, *Journal of Chemistry*, **2015**, 456169, 1-11 (IF=3.21)

319. Isolation, spectroscopic and density functional theory studies of 7-(4-methoxyphenyl)-9h-furo[2,3-f]chromen-9-one: A new flavonoid from the bark of *Millettia ovalifolia*. Taj Ur Rahman, Mohammad Arfan, Tariq Mahmood, Wajiha Liaqat, Mazhar Amjad Gilani, Ghias Uddin, Ralf Ludwig, Khair Zaman, M. Iqbal Choudhary, K.F. Khattak and **Khurshid Ayub***. *Spectrochimica Acta Part A: Molecular and Biomolecular spectroscopy*, **2015**, 146, 24-32 (IF = 4.831)
320. Synthesis, crystal structure, spectroscopic and density functional theory (DFT) study of N-[3-anthracen-9-yl-1-(4-bromo-phenyl)-allylidene]-N-benzenesulfono hydrazine, Muhammad Nadeem Arshad, Abdullah M. Asiri Khalid A. Alamry, Tariq Mahmood, Mazhar Amjad Gilani, **Khurshid Ayub**, Abdulhadi Saleh Birinji. *Spectrochimica Acta Part A: Molecular and Biomolecular spectroscopy*, **2015**, 142, 364-374 (IF = 4.831)
321. Phytochemical, spectroscopic and density functional theory study of diospyrin, and non-bonding interactions of diospyrin with atmospheric gases. Fazl-i-Sattar, Zakir Ullah, Ata-ur-Rahman, Abdur Rauf, Muhammad Tariq, Asif Ali Tahir, **Khurshid Ayub**, Habib Ullah. *Spectrochimica Acta Part A: Molecular and Biomolecular spectroscopy*, **2015**, 141(15), 71-79 (IF = 4.831)
322. Synthesis and properties of 5,7-dihydropyrido[3,2-b:5,6b']diindoles. Tran Quang Hung, Ngo Ngoc Thang, Do Huy Hoang, Tuan Thanh Dang, **Khurshid Ayub**, Alexander Villinger, Stefan Lochbrunner, Gerd-Uwe Flechsig, Peter Langer. *European Journal of Organic Chemistry*, **2015**, 5, 1007-1019 (IF = 3.261)
323. First examples of carbene catalyzed allylation of benzaldehyde with allyltrichlorosilane. Sobia Tabassum, Mazhar Amjad Gilani, **Khurshid Ayub**, Rene Wilhelm, *Journal of the Iranian Chemical Society*. **2015**, 12, 1199-1205 (IF= 2.271)
324. Synthesis, crystal structure and spectroscopic properties of 1,2-benzothiazine derivative: an experimental and DFT Study. Muhammad Nadeem Arshad, Tariq Mahmood, Ather Farooq Khan, Muhammad Zia-Ur-Rehman, Abdullah M. Asiri, Islam Ullah Khan, Riffat Un Nisa, **Khurshid Ayub**, Azam Mukhtar and Muhammad Tariq Saeed. *Chinese Journal of Structural Chemistry*. **2015**, 34 (1), 15-25 (IF = 0.847)
325. Spectroscopic and density functional theory studies of a new rosane type diterpenoid from stachys parviflora, Umar Farooq, **Khurshid Ayub**, Muhammad Ali Hashmi, Rizwana Sarwar, Afsar Khan, Mumtaz Ali. Manzoor Ahmad and Ajmal Khan, *Natural Products Research* **2015**, 29 (9), 813-819 (IF = 2.488)
326. A new rosane type diterpenoid from Stachys parviflora and its density functional theory studies, Umar Farooq, **Khurshid Ayub**, Muhammad Ali Hashmi, Rizwana Sarwar, Afsar Khan, Saleha Suleman Khan, Ajmal Khan, Mumtaz Ali, *Records of Natural Products*, **2015**, 9(3), 329-335 (IF = 2.0)
327. Synthesis and DPPH scavenging assay of reserpine analogues, computational studies and in silico docking studies in AChE and BChE responsible for Alzheimer's disease. Muhammad Yar, Muhammad Arshad, Ariba Farooq, Mazhar Amjad Gilani,

2014

- 328.** Aromaticities of azines relative to benzene; a theoretical approach through the dimethyldihydropyrene probe. Maria, Riffat Un Nisa, Muhammad Hanif, Adeem Mahmood and **Khurshid Ayub***. *Journal of Physical Organic Chemistry*, **2014**, 27(11), 860-866. (IF = 2.155)
- 329.** Doping and dedoping process of polypyrrole: DFT study with hybrid functionals. Habib Ullah, Anwar Ul Haq Ali Shah, Salma Bilal, **Khurshid Ayub***, *Journal of Physical Chemistry C*, **2014**, 118(31), 17819-17830 (IF = 4.177)
- 330.** Palladium catalyzed synthesis and physical properties of Indolo[2,3-*b*]quinoxalines. Tran Quang Hung, Do Huy Hoang, Ngo Ngoc Thang, Tuan Thanh Dang, **Khurshid Ayub**, Alexander Villinger, Aleksej Friedrich, Stefan Lochbrunner, Gerd-Uwe Flechsig, Peter Langer. *Organic & Biomolecular Chemistry*, **2014**, 12(32), 6151-6166 (IF = 3.89)
- 331.** Aromaticity of azines through dyotropic double hydrogen transfer reaction. Maria, Muhammad Hanif, Ralf Ludwig, Tariq Mahmood and **Khurshid Ayub***. *Journal of Molecular Modeling*, **2014**, 20; 2304 (IF = 2.172)
- 332.** Synthesis, characterization and density functional theory study of some new 2-anilinothiazoles. Ayesha Babar, Huma Khalid, **Khurshid Ayub***, Sarah Saleem, Amir Waseem, Tariq Mahmood, Munawar Ali Munawar, Ghulam Abbas and Ather Farooq Khan. *Journal of Molecular Structure* **2014**, 1072, 221-227 (IF = 3.841)
- 333.** Design of liquid crystals with de Vries-like¹ properties: carbosilane-terminated 5-phenylpyrimidine mesogens suitable for chevron-free FLC formulations. Christopher P.J. Schubert, Jan H. Porada, Andreas Bogner, **Khurshid Ayub**, Tamer Andrea, Frank Giesselmann and Robert P. Lemieux. *Journal of Materials Chemistry C*, **2014**, 2, 4581-4589 (IF = 8.067)
- 334.** Spectroscopic and density functional theory studies of 5,7,3',5'-tetrahydroxyflavanone from the leaves of *Olea ferruginea*. Muhammad Ali Hashmi, Afsar Khan, **Khurshid Ayub**, Umar Farooq. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128,225-230. (IF = 4.831)
- 335.** Synthesis of dihydropyrene-cyclophanediene negative photochrome containing internal alkenyl and alkynyl groups and comparison of their photochemical and thermochemical properties. **Khurshid Ayub**, Reginald H Mitchell, *Journal of Organic Chemistry*. **2014**, 79(2), 664-678. (IF = 4.198)
- 336.** Photophysical, electrochemical properties and temperature dependent geometrical isomerism in alkyl quinacridonediimines. Javed Iqbal, **Khurshid Ayub***, Muhammad Nadeem Arshad, Yue Wang, *New Journal of Chemistry*, **2014**, 38, 752 (IF = 3.925)
- 337.** Density functional theory and phytochemical study of pistagremic acid. Habib Ullah, Abdur Rauf, Zakir Ullah, Fazl-i-Sattar, Muhammad Anwar, Anwar-ul-Haq Ali

Shah, Ghias Uddin, **Khurshid Ayub***, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2014**, *118*, 210-214 (IF= 4.831)

2013

- 338.** DFT study of polyaniline NH₃, CO₂ and CO gas sensors: comparison with recent experimental data, Habib Ullah, Anwar-ul-Haq Ali Shah, Salma Bilal and **Khurshid Ayub***, *Journal of Physical Chemistry C*, **2013**, *117*, 23701-23711 (IF =4.177)
- 339.** Copper complexes of bioactive ligands with superoxide dismutase activity. Huma Khalid, Muhammad Hanif, Muhammad Ali Hashmi, Tariq Mahmood, **Khurshid Ayub**, Muhammad Monim-ul-Mehboob, *Mini-Reviews in Medicinal Chemistry*, **2013**, *13*, 1944-1956 (IF = 3.737)
- 340.** Antitussive efficacy and safety profile of ethyl acetate fraction of terminalia chebula, Rizwan Ul Haq, Abdul Wahab, **Khurshid Ayub**, Khalid Mehmood, M. Azhar Sherkheli, Rafeeq Alam Khan, Mohsin Raza. *ISRN Pharmacology*, **2013**, 256934
- 341.** Theoretical insight of polypyrrole ammonia gas sensor. Habib Ullah, **Khurshid Ayub***, Zakir Ullah, Muhammad Hanif, Raziq Nawaz, Salma Bilal, Anwar Ul Haq Ali Shah, *Synthetic Metals*, **2013**, *172*, 14-20 (IF=4.0)
- 342.** The first Zn(II)-catalyzed oxidative amidation of benzylalcohols with alkylamines under solvent-free conditions. Xiao-Feng Wu, Muhammad Sharif, Anahit Pews-Davtyan, Peter Langer, **Khurshid Ayub**, Matthias Beller, *European Journal of Organic Chemistry*, **2013**, *2013*(14), 2783-2787 (IF =3.261)
- 343.** DFT studies of halogen bonding abilities of nitrobenzene with halogens and chlorofluorocarbons. **Khurshid Ayub** and Tariq Mahmood. *Journal of the Chemical Society of Pakistan*, **2013**, *35*(3), 617-620 (IF = 0.698)
- 344.** Density functional theory study of poly(o-phenylenediamine) oligomers. Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub** and Salma Bilal, *Journal of Physical Chemistry C*, **2013**, *117*(8), 4069-4078 (IF = 4.177)
- 345.** Substituents' effect on thermal electrocyclic reaction of dihydroazulene-vinylheptafulvene photoswitch; a DFT study to improve the photoswitch. Nasir Shahzad, Riffat Un Nisa and **Khurshid Ayub***. *Structural Chemistry*, **2013**, *24*, 2115-2126 (IF = 1.795)
- 346.** Synthesis of 4-trifluoromethylpyridines by [5+1] cyclization of 3-hydroxy-pent-4-yn-1-ones with urea. Viktor O. Iaroshenko, Dmytro Ostrovskiy, **Khurshid Ayub**, Anke Spannenberg, Peter Langer. *Advanced Synthesis & Catalysis*, **2013**, *355*, 576-588. (IF= 5.981)

2012

- 347.** Electroclinic effect in axially chiral organosiloxane liquid crystals. V. Jayalakshmi, **Khurshid Ayub**, Robert P. Lemieux, *Ferroelectrics*, **2012**, *431*, 89-98 (IF = 0.695)

- 348.** Pyrrole *versus* quinoline formation in the palladium catalyzed reaction of 2-alkynyl-3-bromothiophenes and 2-alkynyl-3-bromofurans with anilines. A combined experimental and computational study. Ghazwan Ali Salman, Riffat Un Nisa, Vikto O. Laroshenko, Jamshed Iqbal, **Khurshid Ayub**, Peter Langer, *Organic & Biomolecular Chemistry*, **2012**, *10*, 9464-9473. (IF = **3.89**)
- 349.** Synthesis of functionalized indolizines by lewis acid-mediated cyclocondensation of 3-(2-pyridin-2-yl)-propiolates with enones. Verena Specowius, Franziska Bendrath, Marleen Winterberg, **Khurshid Ayub** and Peter Langer. *Advanced Synthesis & Catalysis*, **2012**, *354*, 1163-1169. (IF = **5.981**)
- 350.** Synthesis of 2,6-disubstituted tetrahydroazulene derivatives. Zakir Hussain, Henning Hopf, **Khurshid Ayub** and S. Holger Eichhorn. *Beilstein Journal of Organic Chemistry* **2012**, *8*, 693-698 (IF = **2.544**)

2011

- 351.** Direct observation of diffuse cone behaviour in de vries smectic-a and -c phase. HyungGuen Yoon; Dena M. Agra-Kooijman; **Khurshid Ayub**; Robert P. Lemieux; Satyendra Kumar. *Physical Review Letters* **2011**, *106*, 087801. (IF = **9.185**)
- 352.** Calculation aided synthesis of a very good dihydropyrene negative photochrome and its photochemical properties **Khurshid Ayub**, Rui Li, Cornelia Bohne, Richard Vaughan Williams, Reginald H Mitchell. *Journal of the American Chemical Society*, **2011**, *133*(11), 4040-4045. (IF = **16.383**)

2010

- 353.** Liquid crystals with axially chiral (r)-3,3'-dinitro-2,2',6,6'-tetramethylbiphenyl cores: the lateral shielding effect of bicyclo[2.2.2]octane-1-carboxylate side chains. **Khurshid Ayub**, Mark Moran, Carmen Lazar and Robert P. Lemieux. *Journal of Materials Chemistry*, **2010**, *20*, 6655-6661(Cover story by *Journal of Materials Chemistry* September 2010) (IF = **14.511**)
- 354.** Design of liquid crystals with 'de vries-like' properties: frustration between sma- and smc-promoting elements, Jeffery Roberts, Nadia Kapernaum, Qingxiang Song, Dorothee Nonnenmacher, **Khurshid Ayub**, Frank Giesselmann, Robert P Lemieux. *Journal of the American Chemical Society*, **2010**, *132*, 364-370. (IF = **16.383**)

2008

- 355.** Stable ion NMR and GIAO-DFT study of novel cations from 8,16-Dicyano[2.2]Metacyclophanedienes and from strategically substituted/benzannelated dihydropyrenes: charge-induced tropicity modulation and π switching. Kenneth K

Laali, Takao Okazaki, Reginald H. Mitchell, **Khurshid Ayub**, Rui Zhang, and Stephen G Robinson. *Journal of Organic Chemistry*, **2008**, 73, 456-467. (IF = 4.198)

- 356.** Suppressing the thermal metacyclophadiene to dihydropyrene isomerization-synthesis and rearrangement of 8,16-dicyano[2.2]metacyclophane-1,9-diene and evidence supporting proposed radicaloid mechanism. **Khurshid Ayub**, Rui Zhang, Stephen G. Robinson, Brendan Twamley, Richards V. Williams, Reginald H. Mitchell. *Journal of Organic Chemistry*, **2008**, 73, 451-456. (IF = 4.198)

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Citation = 7000, h-Index 45 i-10 index = 191**

Contributed Conference Presentations

1. “Enhanced static and dynamic nonlinear optical responses of face specific superalkali based alkaline earth complexes of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane” Rehana Bano, Muhammad Arshad, Tariq Mahmood, **Khurshid Ayub**, Ahsan Sharif, Sobia Tabassum, Mazhar Amjad Gilani, **1st International Conferences on Trends and Research in Chemistry, University of Education, Lahore, January 18-19, 2022**
2. “Transition metals incorporated on phosphorene as efficient single atom catalysts for hydrogen evolution reaction: A DFT study” Sonia Iqbal, Khursheed Ahmed,, Ch. Muhammad Fahim Ayaz, Ayesha Khan, **Khurshid Ayub**, Muhammad Hamid Butt, Ahmad Nauman Shah Saqib, Muhammad Ali Hashmi, **1st International Conferences on Trends and Research in Chemistry, University of Education, Lahore, January 18-19, 2022**
3. “Enhanced static and dynamic nonlinear optical responses of face specific superalkali based alkaline earth complexes of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane” Rehana Bano, Muhammad Arshad, Tariq Mahmood, Khurshid Ayub, Ahsan Sharif, Sobia Tabassum , Mazhar Amjad Gilani, **19th International and 31st National Chemistry Conference on Emerging Trends in Chemistry, University of Management and Technology, Lahore, December 16-18, 2021**
4. “A theoretical design of superalkali doped nanocages as high performance nonlinear optical materials” Faiqa Khaliq, Tariq Mahmood, **Khurshid Ayub**, Sobia Tabassum, Mazhar Amjad Gilani, **19th International and 31st National Chemistry Conference on Emerging Trends in Chemistry, University of Management and Technology, Lahore, December 16-18, 2021**

5. "Polypyrrole Based Gaseous Analyte Sensors: An Accurate Comparative Theoretical Study." Hasnain Sajid, Tariq Mahmood, **Khurshid Ayub***, *International workshop on Energy Materials and Nanotechnology*, COMSATS University Islamabad, Abbottabad Campus, August 15-16, 2018
6. "Theoretical Studies of the Ring Opening Polymerization of Cyclic Esters by Yttrium, and Indium Complexes" Riffat Un Nisa, Junnian Wei, **Khurshid Ayub**, and Paula L. Diaconescu. *Organometallic Meeting*, University of California, Los Angeles, December 04, 2016
7. "Benchmark studies of Sc Dimer and DFT approach to Structural and Frequency Analysis of Sc_n (N = 2-14)" Saira Sajjad, Tariq Mahmood, **Khurshid Ayub***, *27th National and 15th International Chemistry Conference*, University of Malakand, August 22-25, 2016,
8. "Benchmarking Studies of Carbon Halogen Bonds by Using Quantum Chemical Methods" Naveen Kosar, Tariq Mahmood, **Khurshid Ayub***, *27th National and 15th International Chemistry Conference*, University of Malakand, August 22-25, 2016
9. "Theoretical Studies for the Sensing Abilities of Polypyrrole to Hydrazine, Uric acid, Sulfonamide and Urea" Hasnain Sajid, Tariq Mahmood, **Khurshid Ayub***, *27th National and 15th International Chemistry Conference*, University of Malakand, August 22-25, 2016.
10. "An accurate Cost Effective DFT Approach to Study Sensor Behavior of Conducting Polymer for Ionic Analytes" Fatima Wasim, Tariq Mahmood, **Khurshid Ayub***, *27th National and 15th International Chemistry Conference*, University of Malakand, August 22-25, 2016.
11. "Acid-Base Chemistry of Polypyrrole" Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub** and Salma Bilal. *Fourth ICS Poster Exhibition*, University of Peshawar, March 12, 2014.
12. "Identification of structural and spectral features of a flavanone isolated from *Olea ferruginea*: A comparative experimental and DFT study" Muhammad Ali Hashmi, Afsar Khan and **Khurshid Ayub**, *Three Days Chemistry Conference*, Hazara University, KPK, Nov 26-28, 2013.
13. "Quantum mechanical investigation on acceleration of electrocyclic reactions through transition metal catalysis" Riffat Un Nisa, Bibi Saima and **Khurshid Ayub***, *Three Days Chemistry Conference*, Hazara University, KPK, Nov 26-28, 2013.

14. "Aromaticity of Azines through Dyotropic Double Hydrogen Transfer Reactions" Maria, Riffat Un Nisa, Bibi Saima, Tariq Mahmood and **Khurshid Ayub***, *Three Days Chemistry Conference, Hazara University, KPK, Nov 26-28, 2013.*
15. "Density Functional Theory Based Study of Poly(o-aminophenol) as a Potential Humidity and Ammonia Gas Sensor" Salma Bibi, Anwar-ul-Haq Ali Shah, Habib Ullah, Salma Bilal* and **Khurshid Ayub**. *Fourth ICS Poster Exhibition, University of Peshawar. March 12, 2014.*
16. "DFT Study of Polyaniline NH₃, CO₂, and CO Gas Sensors: Comparison with Recent Experimental Data" Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub*** and Salma Bilal. *Third ICS Poster Exhibition, University of Peshawar, March 11, 2013,*
17. "Theoretical mechanistic study of the benzoxazole/benzimidazole Synthesis" Raziq Nawaz, **Khurshid Ayub***, *3rd International Symposium on Biomedical Materials: Recent Advances and Challenges. IRCBM Lahore, December 18-20, 2012.*
18. "Thermal Reversion of Cyclophanedienene into Dihydropyrene" Nasir Khan, **Khurshid Ayub*** and Tariq Mahmood, *3rd International Symposium on Biomedical Materials: Recent Advances and Challenges. IRCBM Lahore, December 18-20, 2012.*
19. "Density functional theory (DFT) studies of poly (o-phenylenediamine) (POPD) Oligomer: potential applications in Biosensors" Habib Ullah, **Khurshid Ayub**, Anwar-ul-Haq Ali Shah and Salma Bilal. *3rd International Symposium on Biomedical Materials: Recent Advances and Challenges. IRCBM Lahore, December 18-20, 2012*
20. "Theoretical Insight of Polypyrrole Ammonia Gas Sensor" Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub**, Salma Bilal. *11th International and 23rd National Chemistry Conference, National Centre of Excellence in Physical Chemistry, University of Peshawar, October 15-17, 2012.*
21. "Combined DFT and Semi-empirical Study of Poly (o-Phenylenediamine)" Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub**, Salma Bilal. *11th International and 23rd National Chemistry Conference, National Centre of Excellence in Physical Chemistry, University of Peshawar, October 15-17, 2012.*
22. "Density functional theory study of poly(o-phenylenediamine) Oligomer" Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub** and Salma Bilal, *2nd Symposium on Recent Trends in Indigenous Chemical Research and Awareness on Data Presentation Skills, Baragali Summer Campus, University of Peshawar July 1-5, 2012.*

23. **2nd Symposium on Recent Trends in Indigenous Chemical Research and Awareness on Data Presentation Skills, Baragali Summer Campus, University of Peshawar July 1-5, 2012..**
24. **“Spectroelectrochemical and Computational studies of poly(o-phenylenediamine)”** Habib Ullah, **Khurshid Ayub**, Anwar-ul-Haq Ali Shah and Salma Bilal. **Second ICS Poster Exhibition, University of Peshawar, March 12, 2012.**
25. **“A Combined DFT and Semi-empirical Study of Poly (o-Phenylenediamine): An Oligomers Approach”** Habib Ullah, Anwar-ul-Haq Ali Shah, **Khurshid Ayub** and Salma Bilal. **Second ICS Poster Exhibition, University of Peshawar, March 12, 2012.**
26. **“Structure-Property Relationships in Smectic Liquid Crystals, Molecular Frustration and Layer Contraction.(Poster)”** Robert P. Lemieux, Qingxiang Song, **Khurshid Ayub**, Ian Rugar, Dorothee Nonnenmacher and Frank Giesselmann. **93rd Canadian Chemistry Conference and Exhibition, Toronto, ON, Canada, May 29 – June 2, 2010.**
27. **“Mesogenic Dopants Based on Axially Chiral Dinitrobiphenyl Core (poster)”** **Khurshid Ayub**, Mark Moran, Carman Lazar and Robert P. Lemieux., **The 23rd International Liquid Crystal Conference, Krakow Poland, July 11- 16, 2010.**
28. **“Developing a Rational Design Strategy for “de Vries Like” Liquid crystals (oral presentation)”** Qingxiang Song, **Khurshid Ayub**, Ian Rugar, Nadia Kapernaum, Dorothee Nonnenmacher, Frank Giesselman, Per Rudquist and Robert P Lemieux, **The 23rd International Liquid Crystal Conference, Krakow Poland, July 11- 16, 2010.**
29. **“Diffuse Cone Behavior in a de Vries-type Mesogen with 5-Phenylpyrimidine Core and Organosiloxane Chain (poster)”** HyungGuen Yoon, Dena M. Agra-Kooijman, **Khurshid Ayub**, Robert P. Lemieux, and Satyendra Kumar, **The 23rd International Liquid Crystal Conference, Krakow Poland, July 11- 16, 2010.**
30. **“Improving the Dihydropyrene Photo-switch (oral presentation)”** Richard V. Williams, Reginald H Mitchell and **Khurshid Ayub**. **International Symposium on Novel Aromatics, Luxumberg, July 19-23 2009.**
31. **“Improving the Photochromic Properties of Dihydropyrene Photoswitches by Changing the Internal Substituents. (Poster)”**, **Khurshid Ayub**, Reginald H. Mitchell. **CSC-2008. May 24-28.**
32. **“Improved Photoswitches Based on Dihydropyrene Skeleton. (Poster)”** **Khurshid Ayub**, Reginald H. Mitchell. **ISOP-07, Oct. 7-10, 2007.**

33. “*The Metacyclophanes to Dihydropyrenes Rearrangement, The Nature of the Transition State and Influencing the Ease of Ring Closure.(Poster)*” Reginald H. Mitchell, Richard V. Williams and **Khurshid Ayub**. *ISNA-12, 2007*.
34. “*The Metacyclophanes to Dihydropyrenes Rearrangement, the Nature of the Transition State and Influencing the Ease of Ring Closure.(Lecture)*” Reginald H. Mitchell, Richard V Williams and **Khurshid Ayub**. *Heron Island conference on Reactive Intermediates and Unusual Molecules, 2007*.

Projects Completed

1. “*Computational Design of Cyclophanediene-Dihydropyrene Photoswitches*” (HEC, **2.27 M PKR**)
2. “*Synthesis of New Classes of de-Vries Liquid Crystals based on Bipyrindyl and Pyridyl-Cyclohexyl Cores and their Application in Ferroelectric LCDs*” (CIIT, **0.2 M PKR**)
3. *Tuning the Anticancer Activity of Organometallic Ruthenium(II)-Arene Compounds of Hydroxypyridone Derived Ligands* (HEC, **0.5 M PKR**, startup grant, PI Dr. M. Hanif)
4. “*Thermally Stable Dihydroazulene-Vinylheptafulvene Photoswitches*” (HEC, **1.5 M PKR**)
5. “*Photoswitchable Frustrated Lewis Pairs: Potential Applications in Hydrogen Storage and Catalysis*” (HEC, **3.03M PKR**)
6. “*Are Radical Cations/Anions Potential Modulators of Photoswitching Properties:A theoretical approach*” (HEC Co-Pi **2.2839 M PKR**, PI: Dr Tariq Mahmood)
7. “*Computational Design and Synthesis of Near Infra-red polymethyine Cyanine Dyes and Their Potential Applications as Biomarkers*” (HEC, **2.54 M PKR**, Co-PI, PI: Dr. Tariq Mahmood)
8. “*Non-Linear Properties of Thermally Stable Dihydroazulene-Vinylheptafulvene Photoswitches*” (DSR KFU, Saudi Arabia, **38400 SAR**, Co-PI, PI: Dr. Nadeem Sadiq Sheikh)
9. “*Photo-switchable Frustrated Lewis Pairs; Potential Applicants in Hydrogen Storage*” (DSR KFU, Saudi Arabia, **38400 SAR**, Co-PI, PI: Dr. Nadeem Sadiq Sheikh)

Projects Awarded

1. “*Non-linear Optical Properties of Ttransition Metal Encapsulated Al₁₂N₁₂ Fullerene like Nano-cages* (CIIT, **1.2 M PKR**)
2. “*A Computational Guide to Design High Performance Nonlinear Optical Materials*” (HEC, **6.93 M PKR**, Co-PI, PI: Dr. Mazhar Amjad Gilani)

Projects Submitted

PhD Thesis Supervision

Awarded

1. **Dr. Riffat Un Nisa**, “*Theoretical Mechanistic Investigation of Organic Transformations Catalyzed by Titanium and Zinc*”, COMSATS University Islamabad, Abbottabad Campus (**September 2013- August 2017**)
2. **Dr. Maria**, “*Theoretical Investigations on the Non-Linear Optical (NLO) Properties of Metal Doped $X_{12}Y_{12}$ Nano-cages*”, COMSATS University Islamabad, Abbottabad Campus (**September 2013- August 2017**)
3. **Dr. Bibi Saima**, “*Theoretical Studies on Physical and Chemical Processes of Pristine and Transition Metal Doped Polyaromatic Hydrocarbon*”, COMSATS University Islamabad, Abbottabad Campus (Thesis submitted, **March 2013-February 2020**),
4. **Dr. Sajida Munsif**, “*Theoretical Studies on the Dynamics of Group I and II Elements on/through $(XY)_n$ Nanocages and Nanosheets*”. COMSATS University Islamabad, Abbottabad Campus, (**February 2016- August 2020**)
5. **Dr. Tabish Jadoon**, “*Theoretical Insight into Geometric, Electronic and Sensing Properties of Silver Graphene Composites*”, COMSATS University Islamabad, Abbottabad Campus (Thesis submitted, **September 2015-August 2020**)
6. **Dr. Muhammad Yar**, “*Theoretical Studies on Electrochemical Sensing Applications of Nitrogenated Holey Graphene (C_2N) for Toxic Agents*”. COMSATS University Islamabad, Abbottabad Campus, (**September 2017- December 2020**)
7. **Dr. Bilal Ahmad Farooqi**, *Structural, Electrical and Sensing Ability Study of Polyaniline and its Composites Based on Density Functional Theory*”University of the Punjab, Lahore, (Thesis Submitted, September **2015- February 2021**) **Supervisor I: Dr Umar Farooq**
8. **Dr. Aisha Ashraf**, “*Density Functional Theory Studies on Electrochemical Sensor Properties of Polythiophenes*” University of the Punjab, Lahore (Thesis submitted, **September 2015- February 2021**) **Supervisor I: Dr Umar Farooq**

In Progress

1. Sehrish Sarfaraz, COMSATS University Islamabad, Abbottabad Campus (**February 2021-**)
2. Muhammad Sohaib, COMSATS University Islamabad, Abbottabad Campus (**February 2021-**)
3. Misbah Asif, COMSATS University Islamabad, Abbottabad Campus (**February 2022-**)
4. Annum Ahsan, COMSATS University Islamabad, Abbottabad Campus (**February 2022-**)

PhD Thesis co-supervision

Awarded

1. **Dr. Riaz Hussain**, “*Structural, Electronic and Vibrational properties of 2nd Row Transition Metal Clusters*”, Government College University Faisalabad (2013-2017) **Supervisor: Dr. Abdullah Ijaz**
2. **Dr. Naveen Kosar**, “*Benchmark DFT Approach for Dissociation Energies of Chemically Important Bonds*”, COMSATS University Islamabad, Abbottabad Campus (2015-2019) **Supervisor: Dr Tariq Mahmood**
3. **Dr. Saira Sajjad**, “*Theoretical Investigation on Bonding, Geometrical and Electronic Properties of Transition Metals Clusters and Their Complexes*”, COMSATS University Islamabad, Abbottabad Campus (2013-2019) **Supervisor: Dr Tariq Mahmood**
4. **Dr. Nasir Khan**, “*Improving the Thermal and Spectroscopic Properties of Dihydropyrenes, Fulgides and Spiropyranes through Computational Tools*”. Hazara University, Mansehra, (March 2013-February 2020) **Supervisor: Dr. Wajid Rehman**
5. **Dr. Shahid Hussain**, “*Adsorption of Gaseous Analytes on the Surface of Metal Doped $X_{12}Y_{12}$ ($X= B, Al, Be, Mg$ & $Y= N,P,O$) Nano-cages*” Government College University Faisalabad (September 2015-August 2020) **Supervisor: Dr Shahid Hussain Chatha.**

In Progress

1. **Faizan Ullah**, “*Quantum Chemical Study on Hydrogen Evolution Reaction Through 2D Carbon Surface Supported Single Atom Catalysts*” COMSATS University Islamabad, Abbottabad Campus (2018-Present) **Supervisor: Dr Tariq Mahmood**
2. **Ali Umar**. “*Theoretical Investigation on the Application of 2D Carbon Nitride Surface for Li and Na Ion Batteries*” University of Okara, (2021-Present) **Supervisor: Dr Riaz Hussain**
3. **Fakhar Hussain**. “*DFT study of nonlinear optical response of pure and mixed coinage metal clusters*” University of Okara, (2021-Present) **Supervisor: Dr Riaz Hussain**

MS Thesis Supervised

Completed

1. **Nasir Shahzad**. MS. “*Effect of C-7 Ring Substitution on the Thermal Stability and Absorption Spectrum of Dihydroazulene/Vinylheptafulvene*”, CIIT, Abbottabad Campus (2010-2012)
2. **Maria**, MS “*Measuring Aromaticity of Nitrogenous Bases using Ring Current of Dihydropyrene and Double Hydrogen Transfer Reactions*”, CIIT, Abbottabad Campus (2010-2012)
3. **Riffat Un Nisa**, MS “*Quantum Mechanical Studies on Transition Metal Catalyzed Electrocyclic Reactions*” CIIT, Abbottabad Campus (2011-2013)

4. **Saima Khan**, MS, “*DFT Investigations of Electronic and NLO Properties of Alkali Metals (Li,Na, K) Encapsulated and Surface Decorated Zn₁₂O₁₂ Nano Cages*”, CIIT, Abbottabad Campus (2015-2017)
5. **Zulqarnain Chughtai**, MS, “*Theoretical Insight into Structure, Thermodynamic and Electronic Properties of Polypyrrole/Graphene Composite*”, COMSATS University Islamabad, Abbottabad Campus (2016-2018)
6. **Irum Gul**, MS “*Theoretical Studies on Permeability of Boron and Nitrogen Doped Graphenes for Protium/Deuterium Ions*”, COMSATS University Islamabad, Abbottabad Campus (2016-2018)
7. **Arsalan Ahmed**, MS, “*Theoretical Insight on Permeability of Alkali Metal Ions Through Crown Ether Based Ion Channels*”, COMSATS University Islamabad, Abbottabad Campus (2017-2019)
8. **Sundas Irshad**, MS, “*DFT Investigations on Electronic and Non-Linear Optical Properties of First Row Transition Metals Doped Phosphides Nanocages*”, COMSATS University Islamabad, Abbottabad Campus (2017-2019)
9. **Annum Ehsan**, MS, “*Theoretical Studies on Exploration of Alkaline Earthides and their Non-linear Optical Properties*”, COMSATS University Islamabad, Abbottabad Campus (2017-2019)
10. **Maryam Munir**, MS, “*Theoretical Investigation on the Potential of Polycationic Clusters for the Storage of Light Noble Gases*”, COMSATS University Islamabad, Abbottabad Campus (2017-2019)
11. **Tamseela Bibi**, MS, “*Theoretical Studies of Nonlinear Optical Molecular Switches*” COMSATS University Islamabad, Abbottabad Campus (2018-2020)
12. **Faisal Rafique**, MS, “*Theoretical Insights of Nonlinear Optical Properties in Diradicals and Tetra-Radicals*”, COMSATS University Islamabad, Abbottabad Campus (2017-2020)
13. **Ahmed Bilal**, MS, “*Computational Evaluation of Single Atom Catalyst Adsorbed in Carbon Nitride Surface for Hydrogen Dissociation Reaction*”, COMSATS University Islamabad, Abbottabad Campus (2018-2020)
14. **Ayesha Mukhtar**, MS, “*Theoretical Investigations of Reactions Inside Confined Space of Porous Organic Cages*”, COMSATS University Islamabad, Abbottabad Campus (2018-2020)
15. **Aitazaz Ahsin**, MS, “*Nonlinear Optical Response of Alkali like Superatom Clusters*” COMSATS University Islamabad, Abbottabad Campus (2018-2020)
16. **Akhtar Ali**, MS, “*Nonlinear Optical Properties of Janus Metallides*”, COMSATS University Islamabad, Abbottabad Campus (2017-2020)

17. **Faiza Fayyaz**, MS, “*Impact of Oriented External Electric Field on the Nonlinear Optical Response of Alkaline Earthides; A DFT Study*”, COMSATS University Islamabad, Abbottabad Campus (2019-2021)
18. **Faiza Ahsan** MS, “*NLO Response of Transition Metalide with Alkali Metal as a Source of Excess Electrons – A Theoretical Study*”, COMSATS University Islamabad, Abbottabad Campus (2019-2021)
19. **Iqra Ijaz**, MS, “*Theoretical Studies on NLO Properties of Polaron and Bipolaron States of Conducting Polymer*” COMSATS University Islamabad, Abbottabad Campus (2019-2021)
20. **Maria Asghar**, MS, “*Chiral Recognition through Porous Organic Cages*” COMSATS University Islamabad, Abbottabad Campus (2019-2021)
21. **Uroosa Sohail**, “*Theoretical Studies on Sensing of Transition Metals Using C2N Surface*”, COMSATS University Islamabad, Abbottabad Campus (2020-2022)
22. **Maryium Bibi**, “*DFT Studies of Metal-doped Carbon Rings as Effective Hydrogen Storage Materials*” COMSATS University Islamabad, Abbottabad Campus (2020-2022)
23. **Raheela Bibi**, “*DFT Studies on Nonlinear Optical NLO Response of Transition Metallide Based on Hexaamine*” COMSATS University Islamabad, Abbottabad Campus (2020-2022)

In Progress

1. **Areeg Sajjad**, COMSATS University Islamabad, Abbottabad Campus (September 2021-
2. **Muhammad Aetizaz**, COMSATS University Islamabad, Abbottabad Campus (September 2021-

MS (MPhil) Thesis Co-Supervised

Completed

1. **Habib Ullah**, MPhil, “*Density Functional Theory Study of Electronic and Structural Properties of Polyaniline and Poly(o-Phenylenediamine) Oligomers*”, University of Peshawar, Peshawar (2013) **Supervisor: Dr. Anwar-Ul-Haq Ali Shah**
2. **Raziq Nawaz** MS, “*Theoretical Mechanistic Studies on Cu (II) Catalyzed Synthesis of Benzoxazole and Benzimidazole*” CIIT, Abbottabad Campus, 2013, **Supervisor: Dr. Rehana Rashid**
3. **Huma Khalid**, MS, “*Synthesis and Biological Evaluation of Copper (II) Complexes*” CIIT, Abbottabad Campus, 2013, **Supervisor: Dr. Muhammad Hanif**
4. **Bilal Ahmad Farooqi**, MPhil, “*Density Functional Theory Study of Polyaniline Emeraldine Salt as Chemical Sensor for HBr and HCl*” University of the Punjab, Lahore, 2015, **Supervisor: Dr. Umar Farooq**

5. **Zakir Ullah**, MPhil, “*Density Functional Theory and Experimental Study of Diospyrin and 8-Hydroxydiospyrin*” University of Peshawar, Peshawar, **2015, Supervisor: Dr. Atta-ur-Rehman**
6. **Fazl-i-Sattar**, MPhil, “*Frustrated Lewis Pairs: Metal Free Hydrogen Activation*” University of Peshawar, Peshawar, **2015, Supervisor: Dr. Muhammad Tariq**
7. **Fatima Waseem**, MS, “*Theoretical insight to sensing ability of polypyrrole for nitrogen oxide analytes*” CIIT, Abbottabad Campus, **2016, Supervisor: Dr. Tariq Mahmood**
8. **Hasnain Sajid**, MS, “*Theoretical Studies for the sensing abilities of polypyrrole towards Urea, Uric acid, Acetamide and Sulphonamide*” CIIT, Abbottabad Campus, **2017, Supervisor: Dr. Tariq Mahmood**
9. **Rida Zainab**, MS, “*Theoretical calculations on electrocyclic reactions of radical cations and anions*” CIIT, Abbottabad Campus, **2017, Supervisor: Dr. Tariq Mahmood**
10. **Muhammad Bilal Ahmed Siddiqui**, MPhil, “*Interaction of coronene with silver metal clusters (Ag_n ($n = 2-10$))*”, GC University Faisalabad, **2017, Supervisor: Dr. Sarosh Iqbal**
11. **Saifullah Khan**, MPhil, “*Computational study of Adsorption of Palladium metal clusters (Pd_n ($n = 2-10$)) on Coronene*”, GC University Faisalabad, **2018, Supervisor: Muhammad Saeed**
12. **Faizan Ullah**, MS, “*Quantum Chemical Studies of Non-Linear Optical Properties of Superalkali Doped Phosphide Nanocages*”, COMSATS University Islamabad, Abbottabad Campus, **2018, Supervisor: Dr. Tariq Mahmood**
13. **Sabir Ali Siddiqui**, MPhil, “*Effect of Transition metal (Fe, Co, Ni, Cu and Zn) encapsulation on the hydrogen adsorption efficiency on Boron Phosphide nanocages: A Theoretical Study*”, University of the Punjab, Lahore, **2018, Supervisor: Dr. Muhammad Arshad**
14. **Fatima**, MPhil “*Zinc Oxide clusters adsorption on coronene (ZnO , Zn_2O_2 , Zn_3O_3 , Zn_5O_5 , Zn_6O_6)*” Thesis Submitted, University of Sargodha, **2018, Supervisor:**
15. **Hira Tahir**, MS, “*DFT Investigations of Structural and Nonlinear Optical Properties of Multi-doped Carbon Fullerenes*”, COMSATS University Islamabad, Abbottabad Campus, **2018, Supervisor: Dr. Tariq Mahmood**
16. **Shahnaz Noor**, “*Density Functional Theory and Experimental Studies on Naringenin and 3,5,7,4'-Tetrahydroxy-Flavanone*”, NCEPC, University of Peshawar, Peshawar **2019, Supervisor: Dr. Muhammad Tariq**
17. **Moneeba Asghar** MS, “*Theoretical Studies on Electrochemical Properties of Metal Doped C60 Fullerene for Battery Applications*”, COMSATS University Islamabad, Abbottabad Campus, **2019, Supervisor: Dr. Tariq Mahmood**
18. **Mehwish Qayyum**, MS, “*Synthesis and Investigation of Aggregation Induced Emission Properties of Tetraphenylethylene Analogues*”, COMSATS University Islamabad, Abbottabad Campus, **2019, Supervisor: Dr. Soahil Anjum Shahzad**
19. **Kiran Shehzadi**, MS, “*DFT study of Geometric and Nonlinear Optical Properties of Superalkali Doped Graphdiyne*”, COMSATS University Islamabad, Abbottabad Campus, **2019, Supervisor: Dr. Tariq Mahmood**

20. **Sana Malik**, MS, “*Theoretical Studies on Hydrogen Storage Ability of Zintl Ions*”, COMSATS University Islamabad, Abbottabad Campus, **2017-2019, Supervisor: Dr. Umer Rashid**
21. **Nadia Khan**, MS, “*Theoretical investigation on Radical Anion Promoted Electrocyclization in Photoswitches*”, COMSATS University Islamabad, Abbottabad Campus, **2017-2020, Supervisor: Dr. Tariq Mahmood**
22. **Sidra Khan**, MS, “*Exploration of Structural, Optoelectronic and Aromatic Properties of Helicenes Using DFT Approach*” COMSATS University Islamabad, Abbottabad Campus, **2017-2019, Supervisor: Dr. Tariq Mahmood**
23. **Muhammad Sohaib**, MS, “*DFT Investigations of Fe, Ni, Co and Cu Doped Graphdiyne for Single Atom Catalysis of Oxygen Evolution Reaction*”, COMSATS University Islamabad, Abbottabad Campus, **2018-2020, Supervisor: Dr. Tariq Mahmood**
24. **Tayyaba Murtaza**, MS, “*Theoretical Studies of Electrochemical Properties for Sodium Doped Graphyne Analogs in Battery Applications*” COMSATS University Islamabad, Abbottabad Campus, **2018-, Supervisor: Dr. Tariq Mahmood**
25. **Sameea Ghaffar**, MPhil, “*A Theoretical Study on Structure and Electronic Properties of Iron Oxide-Graphene Nano Clusters*”, University of Sargodha, Sargodha, (In progress, **Fall 2015-. Supervisor:**
26. **Perveen**, MPhil, “*A Theoretical Study on Structure and Electronic Properties of Zinc-Oxide-Graphene Nano Clusters ($n = 7-12$)*”, University of Sargodha, Sargodha, (In progress, **Fall 2015-, Supervisor:**
27. **Ali Tahir**, MPhil, “*DFT studies on hydrogen adsorption ability of alkali and alkaline earth metals encapsulated boron nitride nano cage*”, University of Education DG Khan Campus (In progress, **2017- Supervisor Dr. Riaz Hussain**
28. **Zuhaib Nawaz**, MPhil, “*DFT studies on hydrogen adsorption ability of alkali and alkaline earth metals encapsulated aluminium nitride nano cages*”, Government College University Lahore (In progress, **2018-, Supervisor: Dr. Aziz ur Rehman**
29. **Adnan Aslam**, MPhil, “*Effect of transition metal encapsulation on the hydrogen adsorption efficiency of aluminium nitride nanocages, a theoretical study*”. GC University Faisalabad, (In progress, **2018- Supervisor: Dr Saima Rehman**
30. **Sidra Khan**, MS, COMSATS University Islamabad, Abbottabad Campus, **2018-, Supervisor: Dr. Tariq Mahmood**
31. **Saba Kanwal**, MS, “*DFT Studies on Nonlinear Optical Response of Reversible Thermochromes*” COMSATS University Islamabad, Abbottabad Campus, **2018-, Supervisor: Dr. Tariq Mahmood**
32. **Faiqa Khaliq**, MS, “*Design of Novel Lanthanum Doped Al₁₂P₁₂ Nanocages with High Nonlinear Optical Response*”, COMSATS University Islamabad, Lahore Campus, **2019-2021 Supervisor: Dr. Mazhar Amjad Gilani**

33. **Misbah Asif**, MS, “*Theoretical Studies on Sensing of Pesticide using C4N Nanoflake*” COMSATS University Islamabad, Abbottabad Campus, **2019-2021**, **Supervisor: Dr. Tariq Mahmood**
34. **Sunaina Wajid**, MS, “*Static and Dynamic Hyperpolarizability Analysis of Metal Doped C6O6Li6 Complexes: A DFT Study*” COMSATS University Islamabad, Abbottabad Campus, **2019-2021**, **Supervisor: Dr. Tariq Mahmood**
35. **Laraib Zari**, “*DFT Studies on Nonlinear Optical (NLO) Response of Super Alkali Doped Organometallic Compounds*” COMSATS University Islamabad, Abbottabad Campus, **2020-**, **Supervisor: Dr. Tariq Mahmood**
36. **Sana Qureshi** “*Theoretical Studies on Sensing of Toxic Molecules by using h-g-C3N4 nanoflake*” COMSATS University Islamabad, Abbottabad Campus, **2020-**, **Supervisor: Dr. Tariq Mahmood**

In Progress

Articles Reviewed for

1. Applied Catalysis B: Environment (Elsevier)
2. Chemical Engineering Journal (Elsevier)
3. Journal of Materials Chemistry A (RSC)
4. Journal of Hazardous Materials (Elsevier)
5. ACS Applied Materials and Interfaces (ACS)
6. Advanced Optical Materials (Wiley)
7. Chemosphere (Elsevier)
8. Journal of Materials Chemistry C (RSC Publishing)
9. Journal of Nanostructures in Chemistry (Springer)
10. Inorganic Chemistry Frontiers (RSC)
11. Applied Surface Science (Elsevier)
12. Materials Science and Engineering C (Elsevier)
13. International Journal of Hydrogen Energy (Elsevier)
14. ACS Applied Energy Materials (ACS)
15. Journal of Molecular Liquids (Elsevier)

16. Journal of Alloys and Compounds (Elsevier)
17. Phytotherapy Research (Wiley)
18. Arabian Journal of Chemistry (Elsevier)
19. Catalysis Science and Technology (RSC)
20. Surfaces and Interfaces (Elsevier)
21. Nanomaterials (MDPI)
22. Frontiers in Chemistry (Frontiers)
23. Colloids and Surfaces A; Physicochemical and Engineering Aspect (Elsevier)
24. European Polymer Journal (Elsevier)
25. Polymer Chemistry (RSC)
26. Journal of Molecular Catalysis A: Chemical (Elsevier)
27. Journal of Biomolecular Structure and Dynamics (Taylor and Francis)
28. Measurement (Elsevier)
29. Optics and Laser Technology (Elsevier)
30. Spectrochimica Acta A: Molecular and Biomolecular (Elsevier)
31. Materials Chemistry and Physics (Elsevier)
32. Journal of Saudi Chemical Society (Elsevier)
33. Materials Science in Semiconductor Processing (Elsevier)
34. Energy and Fuels (ACS)
35. ACS Applied Electronic Materials (ACS)
36. Dalton Transaction (RSC Publishing)
37. Results in Physics (Elsevier)
38. Polymer (Elsevier)
39. Journal of Physics and Chemistry of Solids (Elsevier)
40. Zeitschrift Fur Physikalische Chemie (Elsevier)
41. Journal of Traditional and Complimentary Medicines (Elsevier)

42. Journal of Physical Chemistry C (ACS)
43. ACS Omega (ACS)
44. Applied Organometallic Chemistry (Wiley)
45. RSC Advances (RSC Publishing)
46. Synthetic Metals (Elsevier)
47. New Journal of Chemistry (RSC Publishing)
48. Physical Chemistry Chemical Physics (RSC Publishing)
49. Organic and Biomolecular Chemistry (OBC) (RSC publishing)
50. Organic Electronics (Elsevier)
51. Journal of Molecular Structure (Elsevier)
52. Journal of King Saud University Science (Elsevier)
53. Diamond and Related Materials (Elsevier)
54. Computational Biology and Chemistry (Elsevier)
55. Journal of Computational Chemistry (Wiley)
56. Computational Materials Science (Elsevier)
57. Journal of Inorganic and Organometallic Polymers and Materials (Springer)
58. Journal of Chemical Physics (AIP)
59. Journal of cluster Science (Springer)
60. Physica E (Elsevier)
61. Research on Chemical Intermediates (Springer)
62. Applied Biochemistry and Biotechnology (Springer)
63. Journal of Applied Polymer Science (Wiley)
64. Journal of Physical Chemistry A (ACS)
65. Journal of Molecular Graphics and Modeling (Elsevier)
66. Current Applied Physics (Elsevier)
67. Chemical Physics Letters (Elsevier)

68. Optical and Quantum Electronics (Springer)
69. Journal of Solid State Electrochemistry (Springer)
70. Chemical Physics (Elsevier)
71. International Journal of Quantum Chemistry (Wiley)
72. Journal of Organometallic Chemistry (Elsevier)
73. Journal of Sulfur Chemistry (Taylor & Francis)
74. ChemistrySelect (Wiley)
75. Computational and Theoretical Chemistry (Elsevier)
76. Journal of Molecular Modeling (Springer-Verlag)
77. Surface Science (Elsevier)
78. Journal of Heterocyclic Chemistry (Wiley)
79. Synthetic Communications (Taylor & Francis)
80. Journal of the Current Science and Technology
81. Inorganic and Nano-metal Chemistry (Taylor and Francis)
82. International Journal of Modern Physics B (World Scientific)
83. Phosphorus, Sulphur, and Silicon and the Related elements (Taylor & Francis)
84. Russian Journal of Physical Chemistry A (Springer)
85. Journal of the Chemical Society of Pakistan (CSP)
86. Journal of the Indian Chemical Society (Elsevier)
87. Journal of Water and Environmental Nanotechnology
88. SN Applied Sciences
89. Mediterranean Journal of Chemistry
90. Materials Today Proceedings (Elsevier)

Collaborators

1. Prof. Dr. Ralf Ludwig (Germany)
2. Prof. Dr. Victor Yaroshenko (Poland)

3. Dr. Tariq Mahmood (COMSATS, Pakistan)
4. Dr. Mazhar Amjad Gilani (COMSATS, Pakistan)
5. Dr Umar Farooq (Univ. of the Punjab, Pakistan)
6. Dr. Javed Iqbal (UAF, Pakistan)
7. Dr. Nadeem S. S. (University of Brunei)
8. Dr. Riaz Hussain (University of Okara)
9. Dr. Riaz Hussain (University of Education DG Khan)
10. Dr. Ajaz Hussain (BZU, Multan)

References

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