

Curriculum Vitae

Personal Information

Nasarul Islam

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Research Interest

- The research interest of me encompasses broadly **Theoretical Inorganic and Organic chemistry**. During Ph.D. my research focused on the design and development material for OLED and nonlinear devices by means of computational methods. Presently I am interested in performing theoretical investigations over a broad spectrum of systems, ranging from molecules to materials, using a variety of quantum mechanical methods. The main focus of my research is on electronic structure and spectral properties of chiro-optic systems, energy storage and conversion systems, structure-activity relationships and microscopic structure-property relationship for applications based on transport, optical, magnetic and electrical behaviour of condensed systems. The theoretically designed charge transport material for OLED devices displaying good efficiency is then synthesised under laboratory conditions.

Current Position

- **Presently**, I am working as **Assistant Professor** in Higher Education Department Jammu and Kashmir, India from 11th April 2017 to till date.

Education

- Ph. D, awarded on 1st July 2014, titled, "*Theoretical studies on some chiro-optic electronic systems using DFT level of theory*", Department of Chemistry, **University of Kashmir**- India.
- Qualified **NET Examination** two times with 66th and 08th rank conducted by CSIR-UGC, INDIA in June and December 2010 year.
- Master of Science, Department of Chemistry, **University of Kashmir**- India.
- Bachelor of Science, **University of Kashmir**, Srinagar, Kashmir.
- Bachelor of Education, **University of Kashmir**, Srinagar, Kashmir.

Previous Research Positions

- Worked as Dr D. S. **Postdoctoral fellow** under the DSK postdoctoral fellowship scheme (UGC-India) with Prof. S. S. Chimni on the project titled "*SPECTRAL, CHARGE TRANSPORT PROPERTIES AND NONLINEAR OPTICAL RESPONSE OF ORGANO-INORGANIC MATERIAL: A DFT STUDY*" from 23rd Sep. 2014 to 11 April 2017.

- As Ph. D Scholar with Prof. Altaf Hussian Pandith worked on project “*Theoretical studies on some chiro-optic electronic systems using DFT level of theory*” from 28th April 2010 to 1st July 2014.

Previous Teaching Positions

- Worked as contractual lecture in DOIET at **University of Kashmir** for teaching Chemistry to B. Tech Class from 01/05/2013 to 31/12/2013 and 01/05/2014 to 22/09/2014
- Worked as 1st Ph D Scholar in computational chemistry under the supervision of Dr. Altaf Hussain Pandith at Department of Chemistry, **University of Kashmir** w.e.f 28/04/2010.
- Worked as contractual lecture in Space Age Model Higher Secondary Institute Bandipora, for teaching Chemistry to 11th and 12th classes from 01/04/2009 to 30/11/2009

Software/Computer Skills

- ❖ Molecular Modeling: GAUSSIAN 09/03, ORCA, SCHROINDGER, GAMESS R2 2009, VMD, PyMol, AutoDock4.2, ArguesLab, ChemDraw.
- ❖ MD Simulation Package: GROMACS, DESMOND.
- ❖ Computer Languages: FORTRON, C, MATLAB, Python.
- ❖ Document Preparation: LaTeX, MS-Office, BibTeX, Mendeley Desktop, Photoshop, Corel Draw,
Microsoft Office, Adobe Acrobat Professional.
- ❖ Plotting software: Gnuplot, Origin, SYSTAT12
- ❖ Operating Systems: Windows, Linux (Red Hat 5), Centos
- ❖ Others: HTML/CSS, Mathematica, Autodesk Maya (3D graphics software), Bruker- TOPSPIN.

Experimental Techniques and Instruments Used

- Spectroscopic; UV-Vis (Varian, Jasco), Fluorescence (Varian, Perkin Elmer), Circular Dichroism (Jasco), ATR-FTIR (Bruker), Flame Photometry.
- Others; Potentiometer, pH meter and conductometer

Research Activities

Published **34** articles in peer-reviewed journals, **03** articles under revision/submitted, **01** patent, **13** abstracts in international and national conferences and attended **03** workshops.

Published Articles

2017

1. Somenath Panda, Vickramjeet Singh, **Nasarul Islam**, Ramesh Gardas, Understanding ion-ion and ion-solvent interactions in aqueous solutions of NMP based protic ionic liquids through partial molar properties and DFT calculations, *Fluid Phase Equilibria*, 445 (2017) 35-44.
2. **Nasarul Islam** and Altaf Hussain Pandith, A theoretical study of structural, opto-electronic charge Transport properties of Arylboroxine derivatives, Accepted. *Indian J. Phys.* [I. F.: 1.16].
3. Kulwinder Kaur¹, K.J. Singh¹, Vikas Anand, **Nasarul Islam**, Gaurav Bhatia, Namarta Kalia and Jatinder Singh Lanthanide (=Ce, Pr, Nd and Tb) ions substitution at calcium sites of hydroxyl apatite nanoparticles as fluorescent bio probes: Experimental and density functional theory study, *Ceramics International*, (2017) DOI: [10.1016/j.ceramint.2017.05.029](https://doi.org/10.1016/j.ceramint.2017.05.029)
4. **Nasarul Islam** and Altaf Hussain Pandith, *Spectral and nonlinear optical studies of bridged triarylamine heterohelices; A DFT study*, *J. Mol. Struct.* (2017) DOI: [10.1016/j.molstruc.2017.04.030](https://doi.org/10.1016/j.molstruc.2017.04.030) [I.F: 1.78].

5. Rahul Kumar Mudsainiyana, Rajwinder Kaur, **Nasarul Islam**, Amanpreet Kaur Jassal, *Effect of H-bonding interactions of water molecules in the self-assembly of supramolecular architecture- Joint Experimental and Computational studies*, J. Mol. Struct. (2017) DOI: [10.1016/j.molstruc.2017.04.039](https://doi.org/10.1016/j.molstruc.2017.04.039) [I.F: 1.78].
6. **Nasarul Islam** and Swapandeeep Singh Chimni, *Spectral and optoelectronic studies on 7, 12, 17-Trioxa and 7, 12, 17-Trithia [11] helicenes: A DFT view*. Indian J. Phys. DOI: [10.1007/s12648-017-1000-8](https://doi.org/10.1007/s12648-017-1000-8) (in press) [I. F.: 1.16].
7. Jasneet Kaur, **Nasarul Islam**, Akshay Kumar and Swapandeeep Singh Chimni, *Experimental and DFT Studies of Organocatalytic Microwave Assisted Reaction of Isatin Derivatives with Dinitrotoluenes*, Asian J. Org. Chem., DOI: [10.1002/ajoc.201600614](https://doi.org/10.1002/ajoc.201600614) (2017) (in press) [I. F: 3.372] .
8. **Nasarul Islam** and Swapandeeep Singh Chimni, *Geometrical structure and nonlinear response variations of Metal (M= Ni²⁺, Pd²⁺, Pt²⁺) Octaphyrin Complex derivatives; A DFT Study*, J. Coord. Chem. DOI: [10.1080/00958972.2017.1290799](https://doi.org/10.1080/00958972.2017.1290799) (in press) [I. F.: 2.012].
9. **Nasarul Islam**, *Computational studies on optoelectronic and nonlinear properties of Octaphyrin derivatives*. Frontiers in Chemistry DOI: [10.3389/fchem.2017.00011](https://doi.org/10.3389/fchem.2017.00011).

2016

10. **Nasarul Islam** and Swapandeeep Singh Chimni, *Binding and selectivity of phenazino-18-crown-6-ether with alkali, alkaline earth and toxic metal species: A DFT study*, J. Mol. Struct. (2016) [I.F: 1.78] DOI: [10.1016/j.molstruc.2016.10.100](https://doi.org/10.1016/j.molstruc.2016.10.100)
11. Jasneet Kaur, **Nasarul Islam**, Akshay Kumar, Vimal K. Bhardwaj and Swapandeeep Singh Chimni, *Organocatalytic enantioselective synthesis of C₃ functionalized indole derivatives*, Tetrahedron (2016) [I.F: 2.645] DOI: [10.1016/j.tet.2016.10.037](https://doi.org/10.1016/j.tet.2016.10.037)
12. **Nasarul Islam** and Swapandeeep Singh Chimni, *DFT investigation on nonlinear optical (NLO) properties of novel borazine derivatives*, Comp. Theor. Chem. 1086 (2016) 58–66 [I. F: 1.403]
13. Vickramjeet Singh; Pratap Chhotaray; **Nasarul Islam**; Ramesh L Gardas, *Implicit and Explicit Solvent Models to Understand the D(+)-Glucose Solvation in Aqueous Protic Ionic Liquid Solution: Volumetric and Computational approach*, J. Chem. Thermodyn. 103 (2016) 7–16 [I. F: 2.196]. (**highest downloaded paper in last 90 days**)
14. Tabasum Ismail, Syed Shafi, Swarn Singh, Tabasum Sidiq, Anamika Khajuria, Abdul Rouf, Mahipal Yadav, Varma Saikam, Parvinder Pal Singh, Mohammad Sarwar Alam, **Nasarul Islam**, Kalicharan Sharma, Halmuthur Mahabalarao Sampath Kumar, *Synthesis and immunopotentiating activity of novel isoxazoline functionalized coumarins*, Eur. J. Med. Chem. 123 (2016) 90-104 [I. F: 3.902].
15. Naveen Kumar, Akshay Kumar, Jasneet Kaur, **Nasarul Islam**, Swapandeeep Singh Chimni, *Catalyst free Synthesis of 3-Aryl-3-hydroxy-2-oxindole Derivatives using water as solvent: Experimental and DFT studies*, Asian J. Org. Chem., (2016) DOI: [10.1002/ajoc.201600346](https://doi.org/10.1002/ajoc.201600346) [I. F: 3.372].

2015

16. Dharmendra singh, Vickramjeet Singh, **Nasarul Islam**, Ramesh Gardas, *Elucidation of molecular interactions between DBU based protic ionic liquid and organic solvents: thermophysical and computational studies*, RSC Advances, 6 (2016) 623–631 [I. F: **3.82**].
17. **Nasarul Islam** *Investigation of comparative shielding of Morin against oxidative damage by radicals: A DFT study*, Cogent Chemistry (2015), **1: 1078272**, DOI: [10.1080/23312009.2015.1078272](https://doi.org/10.1080/23312009.2015.1078272).
18. Roheena Jan, **Nasarul Islam**, Mohsin Bhat, *Micellar Effect of Ammonium Based Cationic Surfactants on Kinetics of Methylene Blue-Assisted Ru (III) and Cu (II) Catalyzed Cysteine/Cystine Transformation in Acidic Aqueous Media*, J. Surfactants. Deterg, 18 (2015) 855–862 [I. F.: **1.853**].
19. Sozia Ahad, **Nasarul Islam** Altaf Hussain Pandith, *Adsorption studies of Malachite Green on 5-sulphosalicyclic acid doped tetraethoxysilane (SATEOS) composite material*, RSC Advances 5 (2015) 92788-92798 [I. F.: **3.82**].

2014

20. **Nasarul Islam**, Altaf Hussain Pandith, *Analysis of vibrational spectra (FT-IR and VCD) and nonlinear optical Properties of Ruthenium (II) complexes*, J. Coord. Chem., 67 (2014)3288-3310 [I. F: **2.21**]
21. **Nasarul Islam**, A. H. Pandith, *Hole Transport and Non Linear Optical Properties of Triarylamine helicenes; A Theoretical study*, J. Mol. Model., 20:2535 (2014),1-17 [I. F. : **1.98**]
22. **Nasarul Islam**, A. H. Pandith, *Electron Transport and Non Linear Optical Properties of Aryldimesitylboranes: A DFT Study*, PLOS ONE (2014) DOI; **10.1371/journal.pone.0114125** [I. F. : **3.54**]
23. **Nasarul Islam**, Saba Niaz, Taniya Manzoor, and Altaf Hussain Pandith *Theoretical investigations into spectral and non-linear optical properties of brucine and strychnine using Density Functional Theory*, Spectrochim. Acta A, 131 (2014) 461–470. [I. F.: **2.22**]
24. **Nasarul Islam**, Altaf Hussain Pandith, *Vibrational Circular Dichorism and Nonlinear optics of Azobenzene Derivatives; A Theoretical Study*, Int. J. Chem., 3(2014) 184 – 194
25. Saba Niaz, Taniya Manzoor, **Nasarul Islam**, Altaf Hussain Pandith, *Theoretical investigations on Niobium based organometallic system as a potential hydrogen storage system, using Density Functional Theory*, Int. J. Quantum Chem., 114 (2014) 449–457, [I. F.: **2.184**]

2013

26. **Nasarul Islam**, Altaf Hussain Pandith, *Toxicity profile of aromatic derivatives towards Scenedesmus Obliquus; A QSAR study*, Can. J. Chem., 10 (2013) 943-950, [I. F.: **1.242**].
27. **Nasarul Islam**, Altaf Hussain Pandith, *Comparative Assessment of QSTR Models Based on Density Functional, Hartree–Fock, AM1, and PM3 Methods for Acute Toxicity of Aliphatic Compounds Towards Vibrio fischeri*, Int. J. Quantum Chem., 113(2013) 830–839, [I. F: **2.184**].
28. Syed Raashid Maqsood, **Nasarul Islam**, Shabnum Bashir, Badruddin Khan, Altaf Hussain Pandith, *Sigma donor and pi acceptor characteristics of certain NN bidentate ligands: A DFT Study*, J. Coord. Chem., 66 (2013) 2308–2315 [I. F: **2.21**].
29. Suhail-ul-Rehman, **Nasarul Islam**, Syed Zeeshan Fatima and Altaf Hussain Pandith, *Synthesis and Characterization of Sulphosalicylic Acid Doped Tetraethoxysilane Composite Polymer Material By Sol-gel Method*, J. Hazard. Mater. 260 (2013) 313– 322 [I. F: **4.836**].
30. Masarat Maswal, Altaf Hussain Pandith, **Nasarul Islam** and Aijaz Ahmad Dar, *Co-solubilization of the Hydrophobic Drugs Carbamazepine and Nifedipine in Aqueous Nonionic Surfactant Media*J. Solution Chem., 42 (2013)1374–1392 [I. F: **1.256**].

2012 and 2011

31. Altaf Hussain Pandith, **Nasarul Islam**, Zeeshan Fatima Syed, Suhail-ul Rehman, Sateesh Bandaru and Anakuthil Anoop, *Density Functional Theory Prediction of Geometry and VCD Spectra of Bridged Triarylamine Helicenes*, Chem. Phys. Lett., 516 (2011) 199-203 [I. F: **2.280**].
32. Altaf Hussain Pandith, **Nasarul Islam**, *Antimicrobial activity assessment of certain anilide derivatives; a DFT study*, Int. J. Chem., 1 (2012) 71-79.
33. **Nasarul Islam**, Altaf Hussain Pandith, *Modeling of the anti-cancer activity of 1, 4-naphthoquinone derivatives: A theoretical study*, J. Pharm. Res., 5(4), (2012)1846-1853
34. **Nasarul Islam**, Altaf Hussain Pandith, *Modeling of the Toxicity of Chemicals to Hydra attenuata: A DFT Study*, J. Pharm. Res., 5(5) (2012) 2915-2920.

Abstract presented on conferences, workshops and symposiums attended:

1. DFT investigation on chiro-optic studies of bridged triarylamine heterohelicenes, National Conference on nascent innovations in chemical science, SLIET Longowal, Punjab on 21st and 22nd Oct. (**Best Poster Presentation Award**)
2. Attended Arctic MSCA-IF: Symposium organized by UiT The Arctic University of Norway, Tromso, Norway June 1-2, 2016
3. Presented Poster at Vth National Symposium on Advances in Chemical Sciences at Department of Chemistry GNDU, Amritsar Punjab on 2nd and 3rd February 2016.
4. Three day workshop on Drug design, molecular docking, virtual screening and pharmacoinformatics organized by central for Pharmaceutical sciences and natural product in collaboration with Schrodinger INC. USA on Nov. 26-28, 2015 at Central University of Punjab.
5. Workshop on Q-chem at BITS Pilani, 19 October 2015.
6. Presented poster at International conference on nascent developments in chemical sciences: opportunities for academia-industry collaboration, organized by Department of Chemistry, BITS, Pilani from 16-18 October 2015.
7. Electron Transport and Non Linear Optical properties of Aryldimesityl Boranes; A DFT Study (**Best Oral Presentation Award**) 11th JK Science Congress-2015, National, University of Kashmir and DST.
8. Oral Presentation in 21st Conference of NMRS at Guru Nanak Dev University Amritsar -2015.
9. Optoelectronic properties of Ru(II) complexes 4th National symposium on recent Advances in Analytical Science and Applications-Jamia Hamdard, New Delhi. (**Best Poster Presentation Award**)-2015.
10. One Day IUAC Acquaintance Programme on Frontiers in Accelerator based Physics organized by Department of Physics, University of Kashmir and Inter University Accelerator Centre, New Delhi on 24th June -2014.
11. Workshop on chemistry popularization, catalyzed and supported by National council for science and Technology communication, DST, New Delhi-2013.
12. International workshop on Optimizations techniques and software in conjunction with the 46th annual convention of operational research society (ORSI), University of Kashmir. One Day Seminar on open Access Resources Organized by Allama Iqbal Library, University of Kashmir-2012.
13. Electron Transport and Non Linear Optical properties of Aryldimesityl Boranes; A DFT Study (**Best Oral Presentation Award**) 9th JK Science Congress-2013, National, University of Kashmir and DST.
14. Vibrational Circular Dichorism analysis of ephedra molecules; A DFT study, (Best Presentation Award) Chemical Constellation cheminar-2012, An International Conference (**Best Poster Presentation Award**) Department of Chemistry, Dr. B. R. Ambedkar, NIT, Jalandhar
15. Comparative Assessment of QSTR Models based on Density Functional, Hartree-Fock, AMI and PM3 methods for acute toxicity of Aliphatic compounds towards, International Congress on Advances in Human Healthcare systems -2012 (New Delhi, IIT Delhi and Jamia Hamdard).
16. Vibrational Circular Dichorism and Redox analysis of bridged triarylamine heterohelicenes; A DFT study, 8th JK Science congress, National Level-2012. (University of Kashmir and DST).

Member editorial board, scientific committee member and Reviewer:

- Member editorial board in **Frontiers in Applied Chemistry** Science Publishing Group 548 Fashion Avenue, New York, NY 10018, U.S.A.
- Member editorial board in **Journal of Computational Chemistry & Molecular Modelling**, Sift Desk Research Page Fullerton, CA, 92831, United states.
- Scientific committee member
 - Research Member American Chemical Society (30883719)
 - Research Member International Association of Advanced Materials, Sweden (825191911829)
 - Universal Researchers in Environmental & Biological Engineering.
 - Substantial Environmental Engineering and Renewable Energy.
 - Bio-Medical Engineering and Environmental Technology Energy.
- Reviewer

- RSC Advances
- Arabian Journal of Chemistry
- Journal of Coordination Chemistry.
- Journal of Medical and Bioengineering
- Indian Journal of Physics
- Journal of Computational and Theoretical Chemistry

Declaration

I hereby declare that all the information given above is true to the best of my knowledge.



Amritsar, 25th April 2017

(Nasarul Islam)