

Curriculum Vitae

Personal Information

Nasarul Islam

Assistant Professor, Department of Chemistry, HKM-Govt. Degree College
Bandipora-193502, INDIA

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Researchgate ID: : https://www.researchgate.net/profile/Nasarul_Islam

ResearcherID: <http://www.researcherid.com/rid/I-3442-2012>

Web of Science ResearcherID: I-3442-2012

ORCID: <http://orcid.org/0000-0002-5719-0795>

Date of Appointment in Hr. Edu. Dep. J&K: 06-04-2017



Present Address

S/o Mohd Sultan Rather

House No:192

Village: Lowdara,

Post: Bandipora,

District: Bandipora-193502

J&K, INDIA

Office Address

(correspondence)

C/o Department of Chemistry,

HKM-Govt. Degree College,

Bandipora, 193502, J&K, INDIA

Permanent Address

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House No:192

Village: Lowdara,

Post: Bandipora,

District: Bandipora-193502

J&K, INDIA

Research Interest

- My research interest encompasses broadly **Theoretical Inorganic and Organic chemistry**. Using computational approaches, I worked on developing OLED and nonlinear device materials during my Ph.D. I am interested in performing computational investigations over a broad spectrum of systems, ranging from molecules to materials, using various quantum mechanical methods. The main focus of my research is on the 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 synthesized under laboratory conditions.

Current Position & Collaborations

- **Presently**, I am working as an **Assistant Professor** in the Department of Chemistry, HKM-Govt. Degree College Bandipora, J&K, India .
- In my former mentor's group (**Prof. S. S. Chimni**), Department of Chemistry, Guru Nanak Dev University Amritsar, Punjab, we develop and studied mechanisms for transition states and enantioselective origin of products in organocatalyzed reactions.
- I am collaborating with the research group at the Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India for studying the reaction mechanism and molecular dynamic properties of Ionic liquids.

Funded Research Projects Ongoing/Submitted

S. No.	Title of Project	Agency	Duration of Project	Status
1.	Multiscale Computational Studies on Optoelectronic Response of Hetero-structural Fullerene Molecules (MCSOR-HFM)	JKST&IC	2 years (2021-22)	Ongoing
2.	A mathematical and computational model for COVID-19 with special reference to J&K-India	JKST&IC	1 year (2022)	Ongoing

Education

- Ph. D, titled, “*Theoretical studies on some chiro-optic electronic systems using DFT level of theory*”, from Department of Chemistry, **University of Kashmir**- India. Date of Registration, 28-04-2010, **Year of Award, 01-07-2014**
- 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. (2019)
- Bachelor of Science, **University of Kashmir**, Srinagar, Kashmir. (2016)
- Bachelor of Education, **University of Kashmir**, Srinagar, Kashmir. (2010)

Previous Research Positions

- 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*” (2014-2017)
- As **Ph. D Scholar** on the project “*Theoretical studies on some chiro-optic electronic systems using DFT level of theory*” (2010-2014).

Previous Teaching Positions

- Worked as Assistant Professor, Department of Chemistry, Govt. Degree College Sopore-J&K India from 06-06-2017 to 11-05-2020
- Worked as Assistant Professor, Department of Chemistry, Amar Singh College, Srinagar, J&K India from 11-04-2017 to 06-06-2017
- Worked as a contractual lecturer in DOIET at the **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 the Department of Chemistry, the **University of Kashmir** w.e.f 28/04/2010.
- Worked as a contractual lecturer in Space Age Model Higher Secondary Institute Bandipora, for teaching Chemistry to 11th and 12th classes from 01/04/2009 to 30/11/2009

Fellowships and Awards

- **Postdoctoral fellow** under the DSK postdoctoral fellowship scheme (UGC-India) on 01/07/2014
- Received certificate of outstanding contribution in reviewing awarded July 2017 by *Spectrochimica Acta Part A*, Elsevier.
- Received **two best oral and three best poster awards** in international and national conferences.
- 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.

Subjects Taught

- *Theory*
CH-102 (Chemical Bonding); CH-201 (Thermodynamics); CH-303 (Spectroscopy & Photochemistry)
CH-403 (Coordination Chemistry); CH-502 (Quantum Chemistry-I); CH-601 (Material Chemistry)
- *Practical*
CP-201 (Instrumentation Techniques); CP-301 (Inorganic Synthesis); CP- 401 (Modern Analytical Techniques (MAT))

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),

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

Extra-Curricular

- Coordinator Examination at GDC Bandipora from September 2020 till date
- District Coordinator Unnat Bharat Abihyan (Rural development program of Govt of India)

Research Activities

Published **40** articles in peer-reviewed journals, **04** articles under revision/submitted, **15** abstracts in international and national conferences, and attended **03** workshops.

Communicated Articles (2022)

1. Understanding the insight mechanism of organocatalytic Michael addition reaction using DFT calculations-A Review Article (Under Revision)
2. Exploration of Oxindole derivatives as new material for OLEDs: An experimental and A DFT Study (Communicated)
3. Experimental and DFT studies of an organocatalytic enantioselective Friedel-Crafts reaction of sesamol via in situ generated vinylogous imine intermediates (Under Revision)
4. Effect of the anchoring group C20/C30/C60/) on nonlinear optical properties of Indigo systems: A computational studies (Communicated)

Published

2022

1. S. Kaur, J. Kaur, **Nasarul Islam**, A. Anand, Organocatalytic *Synthesis and DFT Study of Versatile Biologically Active Scaffold of Isatyridene Malononitrile Derivatives*, ChemistrySelect, DOI: 10.1002/slct.202203894, [I.F.: 2.33]

2. K. D. Amirchand, V. Singh, **Nasarul Islam**, Volumetric, Compressibility, Spectroscopic, and Theoretical Evaluation of Interactions between Caffeine and Ethanolammonium Butyrate in Aqueous Solutions, *J. Chem. Eng. Data*, DOI: 10.1021/acs.jced.2c00319, [**I.F.:** 3.01]

2021

3. N. Amiri, U. A. Dar, **Nasarul Islam**, M. Guergueb, G. Lemercier, S. Chevreuxd, H. Nasri, *Molecular structure and DFT calculations of aqua(5,10,15,20-tetrakis[4-(benzoyloxy)phenyl] porphyrinato) magnesium-dioxane*, *J. Mol. St.*, DOI:10.1016/j.molstruc.2021.131469, [**I.F.:** 3.648]
4. J. Kaur, B. P. Kaur, **Nasarul Islam**, P. Chauhan, S. S. Chimni, Stereoselective Mannich Reaction of α -Acetoxy- β -keto Esters with Isatin Imine: An Efficient Access to Vicinal Tetra-Substituted Stereocenters, *Eur. J. Org. Chem.*, DOI: 10.1002/ejoc.202101047
5. R. K. Mudsainiyan, Amanpreet Kaur Jassal, **Nasarul Islam**, *Self-assembled H-bonded supramolecular interactions in monomeric complex [Mg(H₂O)₆].L2.2bipy.H₂O; [LH = 2-amino-5-nitrobenzoic acid, bipy = 4,4'-bipyridine]]]: Joint theoretical calculations and Hirshfeld surface analysis*, *J. Mol. St.* 1232, (2021) DOI: 10.1016/j.molstruc.2021.130073 [**I.F.:** 3.648]

2020

6. Umar Ali Dar, **Nasarul Islam**, Shakeel Ahmad Shah, Sunita Salunke Gawali, Quantum Chemical approach towards secondary amino derivatives of C3 substituted Lawsone, *J. Mol. St.* 1203, (2020) DOI: 10.1016/j.molstruc.2019.127306 [**I.F.:** 3.648]

2019

7. Aboothahir Afzal, Mohamed Shahin Thayyil, Renjith Thomas, **Nasarul Islam**, Ajithan Sheena Mary, *Ant-Cancerous Brucine, and Colchicine: Experimental and Theoretical Characterization*; *Chem. Select* DOI: 10.1002/slct.201902698 [**I.F.:** 3.648]

2018

8. Somenath Panda, Vickramjeet Singh, **Nasarul Islam**, Ramesh L. Gardas, *Molecular interactions of choline based ionic liquids with water at different temperatures: An experimental study*; *J. Mol. Liq.* DOI:10.1016/j.molliq.2018.03.027 [**I.F.:** 3.648] (UGC J. No. 24693)

2017

9. **Nasarul Islam** and Swapandeep 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 [**I. F.:** 2.012]. (UGC J. No. 6971)
10. **Nasarul Islam** and Altaf Hussain Pandith, *Chiro-optic, and nonlinear optical studies of bridged triarylamine heterohelices; A DFT study*, *J. Mol. Struct.* (2017) DOI:10.1016/j.molstruc.2017.04.030 [**I.F:** 1.78]. (UGC J. No. 24702)
11. 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 [**I. F.:** 2.473]. (UGC J. No. 17363)
12. 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 hydroxylapatite nanoparticles as fluorescent bio probes: Experimental and density functional theory study*, *Ceramics International*,(2017) DOI: 10.1016/j.ceramint.2017.05.029 [**I. F.:** 2.986]. (UGC J. No. 5336)

13. **Nasarul Islam** and Altaf Hussain Pandith, *A theoretical study of structural, optoelectronic charge Transport properties of Arylboroxine derivatives*, Indian J. Phys [10.1007/s12648-017-1075-2](https://doi.org/10.1007/s12648-017-1075-2) [**I. F:** **1.403**]. (UGC J. No. 20848)
14. 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**] (UGC J. No. 24702).
15. **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**] (UGC J. No. 20848).
16. 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**]. (UGC J. No. 8803)
17. **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). [**I. F:** **3.994**] (UGC J. No. 17722)

2016

18. **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) DOI: [10.1016/j.molstruc.2016.10.100](https://doi.org/10.1016/j.molstruc.2016.10.100) [**I.F:** **1.78**] (UGC J. No. 24702)
19. Jasneet Kaur, **Nasarul Islam**, Akshay Kumar, Vimal K. Bhardwaj, and Swapandeeep Singh Chimni, *Organocatalytic enantioselective synthesis of C₃ functionalized indole derivatives*, Tetrahedron (2016) DOI: [10.1016/j.tet.2016.10.037](https://doi.org/10.1016/j.tet.2016.10.037) [**I.F:** **2.645**] (UGC J. No. 24235)
20. **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**] (UGC J. No. 16462)
21. 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**]. (UGC J. No. 21844) (**highest downloaded paper in last 90 days**)
22. 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**]. (UGC J. No. 28767)
23. 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**] (UGC J. No. 8803).

2015

24. 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**] (UGC J. No. 23625).
25. **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).
26. 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**] (UGC J. No. 10726).
27. 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**] (UGC J. No. 23625).

2014

28. **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**] (UGC J. No. 6971)
29. **Nasarul Islam**, A. H. Pandith, *Optoelectronic, and nonlinear optical properties of triarylamine helicenes: a DFT study*, J. Mol. Model., 20:2535 (2014),1-17 [**I. F.: 1.98**] (UGC J. No. 24697)
30. **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**] (UGC J. No. 37933)
31. **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**] (UGC J. No. 33571)
32. **Nasarul Islam**, Altaf Hussain Pandith, *Vibrational Circular Dichroism and Nonlinear optics of Azobenzene Derivatives; A Theoretical Study*, Int. J. Chem., 3(2014) 184 – 194
33. 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**] (UGC J. No. 23434)

2013

34. **Nasarul Islam**, Altaf Hussain Pandith, *the Toxicity profile of aromatic derivatives towards Scenedesmus Obliquus; A QSAR study*, Can. J. Chem., 10 (2013) 943-950, [**I. F.: 1.242**]. (UGC J. No. 4812)
35. **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**] (UGC J. No. 23434).
36. 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**] (UGC J. No. 6971).
37. 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**] (UGC J. No.28286).
38. 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**] (UGC J. No. 20518).

2012 and 2011

39. 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**] (UGC J. No. 5475).
40. Altaf Hussain Pandith, **Nasarul Islam**, *Antimicrobial activity assessment of certain anilide derivatives; a DFT study*, Int. J. Chem., 1 (2012) 71-79.
41. **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 (UGC J. No. 19169)
42. **Nasarul Islam**, Altaf Hussain Pandith, *Modeling of the Toxicity of Chemicals to Hydra attenuate A DFT Study*, J. Pharm. Res., 5(5) (2012) 2915-2920. (UGC J. No. 19169)

Books Published:

1. **Concise Polymer Chemistry (Book) for BSC and MSc Students Mamta Publications (2019)**

Conferences, workshops & symposiums Organized:

1. Organized a two-day National Symposium at Govt. Degree College Sopore Under the title “ Frontiers in Chemical Science on 4th and 5th Nov. 2017 (**FICS-2017**)

2. Organized online webinars from HKM Degree College Bandipora (2020)
 - I. International Webinar titled “Advanced Nano-Materials for Electronic Sensors” (Date: June 02, 2020, Speaker Dr. Rakesh Kumar, University of Manchester)
 - II. National Webinar titled “Impact of COVID-19 on Mental Health of Youth and its Management” (Date: Jul 16th, 2020, Speaker Dr. Wasim Rashid Kakroo Child and Adolescent Psychologist)
 - III. International Webinar titled “Nanotechnology for Clean Energy Application: Opportunities and Challenges” (Date: Aug 16th, 2020, Speaker Dr. Ahsan Ul Haq Qurashi, KF-University UAE)

Orientation/ Refresh Course attended:

1. Attending one month’s “Summer School on Quantum Information and Quantum Technology (QIQT-2022) organized by DST-India and IISER-Kolkata
2. Attended two weeks Refresh courses on “Data Analysis with Statistical Methods” organized by Ministry of Education-PMMNNTT teaching-learning center, Ramanujan College (University of Delhi), and Indian Accounting Association, NCR Chapter from 21st December 2020-3rd January 2021.
3. Attended TEQIP-III sponsored one-week online short-term course on “Chemistry of Advanced Functional Materials (CAFM-2020)” organized by NIT-Srinagar from 21-25 September 2020.
4. Attended three weeks orientation program organized by IASE Srinagar in 2017.

Invited talk and Abstract presented at conferences, workshops and symposiums attended:

Extension Lecture

1. Presented extension lecture at Khalsa University Amritsar Punjab titled “From Desktop to Benchtop chemistry” on 26th July 2021
2. Presented extension lecture at Rayat-Bahra University Mohali titled “*Computational Calculations in today’s Chemistry*” on 28th Feb. 2018

Invited Talk

3. Delivered Invited talk on NSD-2018 organized by Rayat-Bahra University sponsored by PSCST Chandigarh on 27th Feb. 2018.

Abstracts presented as oral and poster presentations

4. 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. 2016 (**Best Poster Presentation Award**)
5. Attended Arctic MSCA-IF: Symposium organized by UiT The Arctic University of Norway, Tromso, Norway June 1-2, 2016
6. Presented Poster at Vth National Symposium on Advances in Chemical Sciences at Department of Chemistry GNDU, Amritsar Punjab on 2nd and 3rd February 2016.
7. 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. The USA on Nov. 26-28, 2015 at Central University of Punjab.
8. Workshop on Q-chem at BITS Pilani, 19 October 2015.
9. 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.
10. 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.
11. Oral Presentation in 21st Conference of NMRS at Guru Nanak Dev University Amritsar -2015.
12. 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.

13. 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.
14. Workshop on chemistry popularization, catalyzed and supported by the National Council for Science and Technology communication, DST, New Delhi-2013.
15. International workshop on Optimization 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.
16. 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.
17. Vibrational Circular Dichroism 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
18. 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).
19. Vibrational Circular Dichroism and Redox analysis of bridged triarylamine heterohelices; 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
 - The Journal of Physical Chemistry (ACS)
 - RSC Advances
 - Spectrochimica Acta Part A
 - Arabian Journal of Chemistry
 - Journal of Coordination Chemistry.
 - Journal of Medical and Bioengineering
 - Indian Journal of Physics
 - Journal of Computational and Theoretical Chemistry
 - Cogent Chemistry

Declaration

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



Lowdara, 10th July. 2022

(Nasarul Islam)