

CURRICULUM VITAE

Parthapratim Munshi, PhD, FRSC

Professor and Head

Department of Chemistry, School of Natural Sciences,
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🕒 EDUCATION

Doctorate in Crystallography (2005)

Solid State and Structural Chemistry Unit, Chemical Sciences Division,
Indian Institute of Science (IISc.), Bangalore, India

Mentor: Prof. T. N. Guru Row

🕒 EMPLOYMENTS & RESEARCH EXPERIENCES

Professor and Head (July 2021 – present): Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Delhi NCR, UP, **India**.

Associate Professor and Head (July 2018 – June 2021): Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Delhi NCR, UP, **India**.

Assistant Professor (August 2013 – June 2018): Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Delhi NCR, UP, **India**.

Postdoctoral Research Scientist (January 2011 – July 2013): Neutron Scattering Sciences Directorate, Oak Ridge National Laboratory (ORNL), TN, **USA**.

Marie Curie Research Fellow (November 2008 – November 2010): CRM2, Nancy University 1, Nancy, **France**. Host Scientist: Prof. Dr. Christian Jelsch.

Postdoctoral Research Associate (October 2005 – October 2008): School of Chemistry and Biochemistry, University of Western Australia, Perth, **Australia**. Supervisor: Prof. Mark A. Spackman.

🕒 COURSES DEVELOPEMENT AND TEACHING (~ 8 years)

UG Courses: (Since 2013 August)

CHY111: Chemical Principles (Thermodynamics, Chemical Equilibrium & Kinetics)

CHY214: Physical Methods in Chemistry (Crystallography and Thermal Analysis)

CHY342: Chemistry of Solids and Surfaces (Solid State Chemistry and Crystal Chemistry)

PG Courses:

CHY545: Fundamentals of Crystallography (Since August 2013)

BIO521: Structural Biology (Protein crystallography, August 2013 – May 2019)

CHY600: Research Methodology (August 2018 – December 2019)

☉ PROGRAM DEVELOPEMENT

Launched new programs in August 2020 in Chemistry Department at SNU

- Integrated B.Sc.-M.Sc.(Research)
- Integrated B.Sc.-M.Sc.-Ph.D.
- Integrated M.Sc.-Ph.D.
- M.Sc. (Research)

Launching new programs in Chemistry Department at SNU

- Certification (Chemistry Education) Faculty Development Program (Monsoon 2022)
- PG Diploma in Analytical Chemistry (Monsoon 2023)
- Industry Sponsored Ph.D. Program (Spring 2022)

☉ SUPERVISION EXPERIENCES

• Ph.D. Students:

Degree awarded

1. Kunal Kumar Jha, October 2017, Currently, **Senior Research Associate**, Faculty of Chemistry, University of Warsaw, **Poland**. [Web link](#)
2. Suman Kumar Mandal, July 2020, Currently, **Postdoctoral Research Associate**, Bristol BioDesign Institute, School of Chemistry and School of Bio-chemistry, University of Bristol, **UK**. [Web link](#)
3. Sanjay Dutta, April 2021, Currently, **Senior Research Fellow**, Chemistry Department, Shiv Nadar University. **Joining as a Postdoctoral Research Associate** at the Department of Chemistry and Biochemistry, Baylor University, Waco, Texas, **USA**.
4. Saibal Sar, August 2021 (as a co-supervisor), currently at GTZ (India) Pt. Ltd. Kolkata.
5. Surajit Kalita, Thesis submitted in April 2022 (co-supervisor). To join as a postdoctoral research associate in Europe in July 2022.
6. Anil Kumar, Chemistry, Thesis submitted in May 2022. Currently, **Senior Research Fellow**, Chemistry Department, Shiv Nadar University. To join as a postdoctoral research associate in Europe in July 2022.

Continuing

7. Vikas, Thesis to be submitted in December 2022
8. Suchimita Rath, Thesis to be submitted in July 2024
9. Biswajit Mohanty, Thesis to be submitted in December 2024
10. Bijoy Krishna Deka, Thesis to be submitted in August 2025
11. Yogita Gupta, Thesis to be submitted in August 2025

- **M.Sc. Students:**

1. Mr. Vijay Kumar, M.Sc. (from Central University of Gujarat), Thesis in 2016.
2. Ms. Tanya Garain, M.Sc. project continuing, 2021.
3. Mr. Prateek Rai, M.Sc. project continuing, 2021.
4. Ms. Gunjan Gupta, M.Sc. project continuing 2022.

- **B.Sc. Students:**

1. Ms. Srirupa Sen, B.Sc. (Research) Chemistry, Thesis in 2018.
2. Mr. Anindya Menon, B.Sc. (Research) Chemistry, Thesis in 2019.

- **OUR (Opportunity for Undergraduate Research) Students**

1. Mr. Anindya Menon, B.Sc. (Research) Chemistry, 2016-17.
2. Ms. Gunjan Gupta, B.Sc. (Research) Chemistry, 2019-20.
3. Ms. V. Pratishtha Sharma, B.Tech. Computer Science and Engineering, 2019-20 (co-guide)
4. Mr. Aditya Verma, B.Sc. (Research) Chemistry, 2020-21.
5. Ms. Sanjana Maheswari, B.Sc. (Research) Chemistry, 2020-21.
6. Ms. Sowmya S, B.Sc. (Research) Chemistry, 2020-21.

- **SERB funded Project Fellows:**

1. Mr. Ravi Keshri, 2015 – 2017
2. Ms. Preeti Hooda 2018
3. Ms. Arpita Sarma 2021

- **IASc-INSANA-SASI Summer Research Fellow:**

1. Subrat Khamari, 2018
2. Ankita Kundu, 2018

🌀 RESEARCH INTERESTS

- High-resolution single-crystal X-ray and Neutron diffractions, Crystal growth & design, Chemical and biological crystallography, Materials characterizations and Charge density analysis
- Organic optical, semiconductor, ferroelectric, piezoelectric & pyroelectric, and thermo-responsive materials (negative thermal expansion), optoelectronic devices, polymorphism, biologically active compounds and drug development

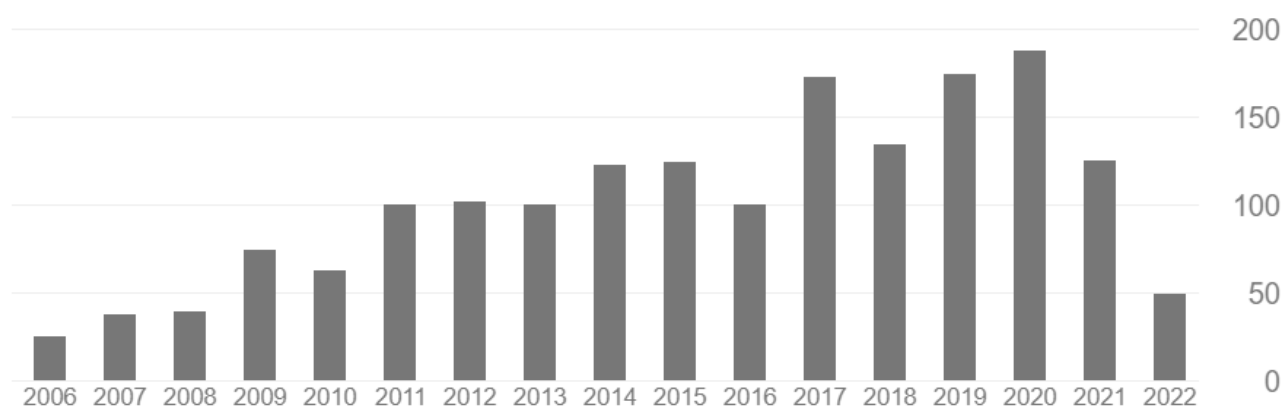
- Protein charge density analysis, Protein-ligand interactions, Molecular docking and interaction energy studies
- Hydrogen bonding and intermolecular interactions, Molecular modelling, Computational chemistry, Quantum Crystallography

🔗 RESEARCH PUBLICATIONS

Total Number: ~70

Citation Indices: (<http://scholar.google.com/citations?user=F-FtnEQAAAAAJ>)

	All	Since 2017
Citations	1774	844
h-index	24	18
i10-index	36	32



1. A. Kumar, J. Chauhan, K. Dubey, S. Sen, **P. Munshi***, "Tuning Potency of Bioactive Molecules via Polymorphic Modifications: A Case Study", *Mol. Pharmaceutics*, **2022**, 19(3), 1008–1018.
2. S. Dutta, Vikas, T. Vijayakanth, R. Boomishankar and **P. Munshi***, "Ferroelectricity and negative thermal expansion in a purely organic single-component material." *ACS Appl. Electron. Mater.* **2021**, 3(8), 3633–3640.
3. S. K. Mandal and **P. Munshi*** "Predicting Accurate Lead Structures for Screening Molecular Libraries: A Quantum Crystallographic Approach" *Molecules* **2021**, 26(9), 2605-2621.
4. S. Dutta and **P. Munshi*** "Unusual Anisotropic Thermal Expansions with Reversible Axial Switching and Record-Wide Thermal Hysteresis in Single-Component Purely Organic Molecular Crystals" *J. Phys. Chem. C.*, **2020**, 124, 27413 - 27421.

5. S. K. Mandal, B. Guilot, **P. Munshi*** "*Electron Density Based Analysis of N-H...O=C Hydrogen Bonds and Electrostatic Interaction Energies in High-resolution Secondary Protein Structures: Insights from Quantum Crystallographic Approaches*" *CrystEngComm*, **2020**, 22, 4363-4373.
Note: This work has been published as a "Cover page (back)" in *CrystEngComm*, 2020, **22**, 4501.
6. S. K. Mandal, **P. Munshi**, "Predicting Lead Structure(s) for Molecular Library Screening Using Molecular Docking and Quantum Crystallography", SSRN 3532904, **2020**.
7. S. Dutta, Vikas, A. Yadav, R. Boomishankar, A. Bala, V. Kumar, T. Chakraborty, S. Elizabeth, and **P. Munshi*** "*Record-high Thermal Stability Achieved in a Novel Single-Component All-organic Ferroelectric Crystal Exhibiting Polymorphism*" *Chem. Commun.* **2019**, 55, 9610-9613.
Note: This work has been published as a "Cover page (inside)" in *Chem. Commun.* **2019**, 55, 9572.
8. K. K. Jha, Y. Yadav, S. B. Srivastava, D. Chakraborty, P. Johari, S. P. Singh and **P. Munshi*** "Structure-property Relationship in an Organic Semiconductor: Insights from Energy Frameworks, Charge Density Analysis and Diode Device" *Cryst. Growth Des.* **2019**, 19(5), 3019-3029.
9. K. K. Jha, S. Dutta, S. Sar, S. Sen, and **P. Munshi*** "Harnessing *Sun* for Catalyst and Sensitizer Free Regio- and Stereo-selective [2+2] Cycloaddition" *Tetrahedron*, **2018**, 74(51), 7326-7334.
10. A. Iruthayaraj, K. Chinnasamy, K. K. Jha, M. S. Pavan, **P. Munshi**, and P. Kumaradhas "Topology of electron density and electrostatic potential of HIV reverse transcriptase inhibitor zidovudine from high resolution X-ray diffraction and charge density analysis" *J. Mol. Struc.*, **2018**, 1180, 683-697.
11. D. Jayatilaka*, K. K. Jha and **P. Munshi*** "Is it reasonable to obtain information on the polarizability and hyperpolarizability from the electron density?" *Aust. J. Chem.* **2018**, 71(4) 295-306.
12. K. K. Jha, S. Dutta, and **P. Munshi*** "Concomitance, reversibility and switching ability of centrosymmetric and non-centrosymmetric crystal forms: Polymorphism in an organic NLO material" *Cryst. Growth Des.* **2018**, 18(2), 1126-1135.
Note: This article has been selected as a Highlighted article - Editor's choice.
13. G. Singh, P. Kalra, A. Arora, A. Singh, G. Sharma, I. K. Maurya, S. Dutta, **P. Munshi**, V. Verma "Acetylenic Indole-Encapsulated Schiff Bases: Synthesis, In Silico Studies as Potent Antimicrobial Agents, Cytotoxic Evaluation and Synergistic Effects" *ChemistrySelect*, **2018**, 3(8), 2366-2375.
14. S. K. Mandal, P. Saha, **P. Munshi***, N. Sukumar "Exploring Potent Ligand for Proteins: Insights from Knowledge-based Scoring Functions and Molecular Interaction Energies", *Structural Chemistry*, **2017**, 28(5), 1537-1552.
15. V. Kumar, R. Thaimattam, S. Dutta, **P. Munshi**, A. Ramanan "Structural landscape of multicomponent solids based on sulfa drugs", *CrystEngComm*, **2017**, 19, 2914-2924.
16. K. K. Jha, S. B. Srivastava, S. P. Singh and **P. Munshi*** "Efficient organic NLO material: charge-density analysis and device fabrication" *Acta Cryst.* **2017**, A73, C800.

17. S. K. Mandal, B. Guillot and **P. Munshi*** "Topological analysis of hydrogen bonds and interaction energies in proteins" *Acta Cryst.* **2017**, A73, C573.
18. S. Dutta, A. Menon and **P. Munshi*** "Exploring ferroelectricity in organic salts or co-crystals" *Acta Cryst.* **2017**, A73, C726.
19. E. Sangtani, K. Jha, **P. Munshi** and R. Gonnade "Co-crystals/salts of furosemide: interesting case of colour co-crystal polymorphism" *Acta Cryst.* **2017**, A73, C724.
20. **P. Munshi*** "Charge-density studies in small molecules and proteins: sources and detectors" *Acta Cryst.* **2017**, A73, C1387.
21. E. Sangtani, S. K. Mandal, A. S. Sreelakshmi, **P. Munshi**, R. Gonnade "Salts and Cocrystals of Furosemide with Pyridines: Differences in π -Stacking and Color Polymorphism". *Crystal Growth & Design*, **2017**, 17 (6), 3071–3087.
22. N. Kumar, S. Hati, **P. Munshi**, S. Sen, S. Sehrawat, S. Singh "A novel spiroindoline targets cell cycle and migration via modulation of microtubule cytoskeleton" *Molecular Cell Biochemistry*, **2017**, 429(1-2), 11-21.
23. P. K. Dutta, A. Majumder, S. Dutta, B. B. Dhar, **P. Munshi**, S. Sen," Solvent free, palladium catalyzed highly facile synthesis of diaryl disulfides from aryl thiols" *Tetrahedron Letter*, **2017**, 58, 527-530.
24. K. K. Jha, S. Dutta, V. Kumar, **P. Munshi***, "Isostructural Polymorphs: Qualitative Insights from Energy Frameworks" *CrystEngComm*, **2016**, 18, 8497-8505.
25. S. Hati, P. Kumar Dutta, S. Dutta, **P. Munshi**, S. Sen, "Accessing Benzimidazoles via a Ring Distortion Strategy: An Oxone Mediated Tandem Reaction of 2-Aminobenzylamines" *Organic Letter*, **2016**, 18 (13), 3090-3093.
26. C. Bathula, S. Tripathi, R. Srinivasan, K. K. Jha, A. Ganguli, G. Chakrabarti, S. Singh, **P. Munshi**, S. Sen "Synthesis of novel 5-arylidene-thiazolidinones with apoptotic properties via a three component reaction using piperidine as a bifunctional reagent" *Organic & Biomolecular Chemistry*, **2016**, 14, 8053-8063.
27. R. Mamidala, P. Majumdar, K. K. Jha, C. Bathula, R. Agarwal, M. T. Charya, H. Mazumdar, **P. Munshi**, S. Sen, "Identification of Leishmania donovani Topoisomerase 1 inhibitors via intuitive scaffold hopping and bioisosteric modification of known Top 1 inhibitors". *Scientific Report*, **2016**, 6, 28120.
28. E. Sangtani, S. K. Sahu, S. H. Thorat, R. L. Gawade, K. K. Jha, **P. Munshi**, R. Gonnade "Furosemide Cocrystals with Pyridines: An Interesting Case of Color Co-crystal Polymorphism". *Crystal Growth & Design*, **2015**, 15, 5858 - 5872.
29. C. Bathula, P. Dangi, S. Hati, R. Agarwal, **P. Munshi**, S. Singh, S. Sen "Diverse synthesis of natural product inspired fused and spiro-heterocyclic scaffolds via ring distortion and ring construction strategy" *New Journal of Chemistry*, **2015**, 39, 9281.

30. C. Bathula, R. Mamidala, C. Thulluri, R. Agarwal, K. K. Jha, **P. Munshi**, U. Adepally, A. Singh, M. Thirumalachary, S. Sen “Substituted furopyridinediones as novel inhibitors of α -glucosidase”. *RSC Advances*, **2015**, 5, 90374.
 31. A. C. Shaikh, D. S. Ranade, S. Thorat, A. Maity, P. P. Kulkarni, R. G. Gonnade, **P. Munshi** and N. T. Patil "Highly Emissive Organic Solids with Remarkably Broad Color Tunability Based on N, C-Chelate Four-Coordinate Organoborons". *ChemComm*, **2015**, 51, 16115.
 32. B. Zarychta, A. Lyubimov, M. Ahmed, **P. Munshi**, B. Guillot, A. Vrielink, C. Jelsch. “Ultra-high resolution crystal structure and charge density study of cholesterol oxidase”. *Acta Crystallographica Section D*, **2015**, 71, 954.
 33. G. Prabhu, S. Agarwal, V. Sharma, S. M. Madurkar, **P. Munshi**, S. Singh, S. Sen. “A natural product based DOS library of hybrid systems” *European Journal Medicinal Chemistry*, **2015**, 95, 41.
 34. **P. Munshi**, E. Snell, M. van der Woerd, R. Judge, D. Myles, Z. Ren, F. Meilleur, “Neutron structure of the cyclic glucose bound Xylose Isomerase E186Q mutant.” *Acta Crystallographica Section D*, **2014**, 70, 414.
 35. **P. Munshi*** & K. K. Jha “Exploring Charge Transfer Mechanism in Organic NLO (Polymorphic) Materials”, *Acta Crystallographica Section A*, **2014**, 70, C378.
 36. **P. Munshi**, C. B. Stanley, S. Ghimire-Rijal, Xun Lu, D. A. Myles, M. J. Cuneo, “Molecular detail of ligand selectivity determinants in a promiscuous β -glucan periplasmic binding protein.” *BMC Structural Biology*, **2013**, 13:18.
- Note:** This article has been selected as *highly accessed* article.
37. F. Meilleur, **P. Munshi**, L. Robertson, A. Stoica, L. Crow, A. Kovalevsky, T. Koritsanszky, B. C. Chakoumakos, R. Blessing, D. A. A. Myles, “IMAGINE: first neutron protein structure and new capabilities for neutron macromolecular crystallography.” *Acta Crystallographica Section D*, **2013**, 69, 2157 - 2160.
 38. **P. Munshi**, S-L. Chung, M. P. Blakely, K. Weiss, D. A. Myles, F. Meilleur, “Rapid visualization of hydrogen positions in protein neutron crystallography structures.” *Acta Crystallographica Section D*, **2012**, 68, 35 - 41.
- Note:** This article has been selected as *Highlighted Article* in the *IUCr News Letter*.
39. V. Hathwar, R. G. Gonnade, **P. Munshi**, M. M. Bhadbhade, T. N. Guru Row, “Halogen bonding in 2, 5-dichloro-1, 4-benzoquinone: Insights from experimental and theoretical charge density analysis.” *Crystal Growth & Design*, **2011**, 11(5), 1855 - 1862.

40. S. Domagala, **P. Munshi**, M. Ahmed, B. Guillot, C. Jelsch, “Structural analysis and multipole modelling of quercetin monohydrate – A quantitative and comparative study.” *Acta Crystallographica Section B*, **2011**, 67, 63 - 78.

Note: This article has been selected as *Highlighted Article* in the *IUCr News Letter*.

41. (a) **P. Munshi**, C. Jelsch, V. Hathwar, T. N. Guru Row, “Experimental and Theoretical Charge Density Analyses on Polymorphic Structures: A Case of Coumarin 314 dye.” *Crystal Growth & Design*, *10*(4), **2010**, 1516-1526. (b) *Corrections*, *10*(10), **2010**, 4670.
42. D. Jayatilaka, **P. Munshi**, M. Turner, J. A. K. Howard, M. A. Spackman, “Refractive indices for molecular crystals from the response of X-ray constrained Hartree–Fock wavefunctions.” *Physical Chemistry Chemical Physics*, *11*, **2009**, 7209-7218.
43. **P. Munshi**, B. Guillot, D. Liebschner, C. Jelsch, Quantitative analysis of atomic polarization in protein human aldose reductase. *Acta Crystallographica Section A*, *65*, **2009**, s172.
44. C. Jelsch, S. Domagala, B. Zarychta, C. Lecomte, B. Guillot, **P. Munshi**, Assessment of electron density refinement quality using free *R*-factors and restraints. *Acta Crystallographica Section A*, *65*, **2009**, s76.
45. **P. Munshi**, A. O. Madsen, M. A. Spackman, S. Larsen and R. Destro, “Estimated hydrogen anisotropic displacement parameters: A comparison between different methods and with neutron diffraction results.” *Acta Crystallographica Section A*, *64*, **2008**, 465-475.

Note: This article has been selected as *Highlighted Article* in the *IUCr News Letter*.

46. **P. Munshi**, B. W. Skelton, J. J. McKinnon, and M. A. Spackman, “Polymorphism in 3-methyl-4-methoxy-4'-nitrosilbene, A Highly Active NLO Material.” *CrystEngComm*, *10*, **2008**, 197-206.
47. **P. Munshi**, B. Dittrich, M. A. Spackman, D. Jayatilaka, and L. H. Rees, Estimation of optical properties from wavefunction fitting of X-ray diffraction data. *Acta Crystallographica Section A*, *64*, **2008**, C128.
48. M. M. Bhadbhade, R. G. Gonnade, **P. Munshi**, T. N. Guru Row, Charge density studies on halogen bonding interactions. *Acta Crystallographica Section A*, *64*, **2008**, C568.
49. M. A. Spackman, **P. Munshi** and D. Jayatilaka, “The Use of Dipole Lattice Sums to Estimate Electric Fields and Dipole Moment Enhancement in Molecular Crystals.” *Chemical Physics Letters*, *443*, **2007**, 87-91.
50. M. A. Spackman, **P. Munshi** and B. Dittrich, “Dipole Moment Enhancement in Molecular Crystals from X-ray Diffraction Data.” (*mini review*). *A European Journal of Chemical Physics and Physical Chemistry*, *8*, **2007**, 2051-2063.

51. B. Dittrich, **P. Munshi** and M. A. Spackman, Redetermination, Invariom-model and Multipole Refinement of L-orthinine Hydrochloride. *Acta Crystallographica Section B*, 63, **2007**, 505-509.
52. **P. Munshi**, E. M. Cameron, J. D. Ferrara, T. N. Guru Row, and T. S. Cameron, Investigation of Inter-ion Interactions in N,N,N'N'-tetramethylethlenediammonium dithiocyanate via Experimental and Theoretical Charge Density Studies. *The Journal of Physical Chemistry A*, 111(32), **2007**, 7888-7897.
53. B. Dittrich, **P. Munshi** and M. A. Spackman, Invariom-model Refinement of L-valinol. *Acta Crystallographica Section C*, 62, **2006**, o633-o635.
54. **P. Munshi** & T. N. Guru Row, Intra and Intermolecular Interactions in Small Bioactive Molecules: Cooperative Features from Experimental and Theoretical Charge Density Analysis. *Acta Crystallographica Section B*, 62, **2006**, 612-626.
55. **P. Munshi** & T. N. Guru Row, Topological Analysis of Charge Density Distribution in Concomitant Polymorphs of 3-acetylcoumarin, A Case of Packing Polymorphism. *Crystal Growth & Design*, 6(3), **2006**, 708-718.
56. **P. Munshi**, T. S. Thakur, T. N. Guru Row, and G. R. Desiraju, Five Varieties of Hydrogen Bonds in 1-Formyl-3-Thiosemicarbazide. An Electron Density Study. *Acta Crystallographica Section B*, 62, **2006**, 118-127.
57. **P. Munshi** & T. N. Guru Row, Charge Density Based Classification of Intermolecular Interactions in Molecular Crystals. *CrystEngComm*, 7(100), **2005**, 608-611.
58. **P. Munshi** & T. N. Guru Row, Evaluation of Intermolecular Interactions in Molecular Crystals via Experimental and Theoretical Charge Densities. *Crystallography Reviews*, 11(3), **2005**, 199-241.
- Note:** This publication is an invited *Review*.
59. **P. Munshi** & T. N. Guru Row, Exploring the Lower Limit in Hydrogen Bonds: Analysis of Weak C-H...O and C-H... π Interactions in Substituted Coumarins from Charge Density Analysis. *The Journal of Physical Chemistry A*, 109(4), **2005**, 659-672.
60. **P. Munshi** & T. N. Guru Row, Topological analysis of charge densities in polymorphs of 3-acetylcoumarin. *Acta Crystallographica Section A*, 61, **2005**, C423-C424.
61. T. S. Cameron, E. M. Cameron, J. D. Ferrara, T. N. Guru Row, and **P. Munshi**, Examination of all inter-ion interactions in $(\text{CH}_3)_2\text{N}(\text{H})\text{CH}_2\text{CH}_2\text{N}(\text{H})(\text{CH}_3)_2(\text{SCN})_2$. *Acta Crystallographica Section A*, 61, **2005**, C428.
62. **P. Munshi** & T. N. Guru Row, 2H-Thiochromene-2-thione. *Acta Crystallographica Section E*, 60, **2004**, o2168.

- 63. P. Munshi**, K. N. Venugopala, B. S. Jayashree, and T. N. Guru Row, Concomitant Polymorphism in 3-acetylcoumarin: Role of Weak C-H...O and C-H... π Interactions. (*Commun*). *Crystal Growth & Design*, 4(6), **2004**, 1105-1107.
- 64. (a) P. Munshi** & T. N. Guru Row, Electron Density Study of 2H-chromene-2-thione. *Acta Crystallographica Section B*, 58, **2002**, 1011-1017. **(b)** 59, **2003**, 159.
- 65. P. Munshi** & T. N. Guru Row, 2H-Thiochromene-2-one. *Acta Crystallographica Section E*, 58, **2002**, o353.
- 66. P. Munshi** & T. N. Guru Row, Experimental charge density analysis on modified coumarins: topological properties. *Acta Crystallographica Section A*, 58, **2002**, C354.
- 67. P. Munshi** & T. N. Guru Row, 2H-Chromene-2-thione. *Acta Crystallographica Section E*, 57, **2001**, o1175.

Book Chapter

- 68. S. Mandal and P. Munshi*** “Charge Density Studies and Topological Analysis of Hydrogen Bonds in Proteins” in “*Understanding Intermolecular Interactions in the Solid State: Approaches and Techniques*”, ed. D. Chopra, Royal Society of Chemistry, UK, 1st edn, **2018**, vol. 1, Chapter 6, Print ISBN: 978-1-78801-079-5.

Other Publications

- 69. C. Bathula, S. Tripathi, R. Srinivasan, K. K. Jha, A. Ganguli, G. Chakrabarti, S. Singh, P. Munshi, S. Sen** “ChemInform Abstract: Synthesis of Novel 5-Arylidene-thiazolidinones with Apoptotic Properties via a Three Component Reaction Using Piperidine as a Bifunctional Reagent.” *ChemInform*, **2016**, 47(52), DOI: 10.1002/chin.201652261.
- 70. S. Hati, P. Kumar Dutta, S. Dutta, P. Munshi, S. Sen**, “ChemInform Abstract: Accessing Benzimidazoles via a Ring Distortion Strategy: An Oxone Mediated Tandem Reaction of 2-Aminobenzylamines” *ChemInform*, **2016**, 47(46), DOI: 10.1002/chin.201646135.
- 71. P. Munshi, S.-L. Chung, M. P. Blakely, K. Weiss, D. A. Myles, F. Meilleur**, Rapid visualization of hydrogen positions in protein neutron crystallography structures. *IUCr. News Letter*, **2012**, Vol 20.
- 72. S. Domagala, P. Munshi, M. Ahmed, B. Guillot, C. Jelsch**, Structural analysis and multipole modelling of quercetin monohydrate – A quantitative and comparative study. *IUCr. News Letter*, **2011**, Vol 19 (1).
- 73. P. Munshi, A. O. Madsen, M. A. Spackman, S. Larsen and R. Destro**, Estimated hydrogen anisotropic displacement parameters: A comparison between different methods and with neutron diffraction results. *IUCr. News Letter*, **2008**, Vol 16 (3).

74. **P. Munshi** & T. N. Guru Row, "ChemInform Abstract: Evaluation of Intermolecular Interactions in Molecular Crystals via Experimental and Theoretical Charge Densities." *ChemInform*, **2006**, 37(34), DOI: 10.1002/chin.200634300.
75. **P. Munshi** & T. N. Guru Row, Charge density analysis on molecular crystals via accurate X-ray diffraction data. *ICA. News Letter*, **2005**, Vol 1.

☉ RESEARCH GRANTS (As only PI)

Funding Agency: SERB/DST/EMR

Project Title: Quantitative Studies of Hydrogen Bonding and Electrostatic Interaction Energies in Proteins: Insights from Advanced Charge Density Analysis

Duration: 2015-2018 (completed)

Amount: 53 Lakhs

Funding Agency: SERB/DST/CRG

Project Title: Exploring Ferroelectricity in Single-component Organic Molecular Crystals: Cases of Imidazole

Duration: 2019 – 2022 (ongoing)

Amount: 32.3 Lakhs

Funding Agency: Bragg Institute, Australian Nuclear Science and Technology Organisation

Project Title: Exploring Charge Transfer Mechanism in Organic NLO (Polymorphic) Materials: Insights from Charge Density Analysis

Duration: May 11 - 16, 2015.

Amount: Neutron beam time worth 20 Lakhs

☉ AWARDS & FELLOWSHIPS

- **Research Excellence Award** by Shiv Nadar University, **2021**.
- **Fellow of Royal Society of Chemistry (FRSC)**, London, UK, **2020**.
- **Emerging Investigators in Crystal Growth & Design – An ACS journal**, **2019**.
- **International Travel Support** from SERB-DST, India Govt. July **2005**, July **2014** and June **2018**.
- **Research grant of 53Lakhs Rupees** from SERB-DST, India Govt. **2015**.
- **Significant Event Award** from ORNL for exceptional teamwork for the commissioning of IMAGINE beam line, **2013**.
- **Travel Fellowship Awards** from the U.S. National Committee for the IUCr. Aug. **2011**.
- **Selected** for the 2nd Annual Young Investigators' Meeting (YIM) Boston, USA, Oct. **2010**.
- **Postdoctoral fellowship** at the Oak Ridge National Laboratory, TN, USA, Jan. **2011**.
- **Qualified** in a global competition among young scientists worldwide to participate in the 60th **Meeting of Nobel Laureates** at Lindau, Germany, Jun / Jul **2010**.

- **Marie Curie International Incoming Fellowship** within the 7th European Community Framework Programme, France, Nov 2008 – Oct **2010**.
- **Postdoctoral fellowship** at the University of Western Australia, WA, Perth, Australia, Oct. **2005**.
- **Senior Research Fellowship**, Council of Scientific and Industrial Research, India **2003 – 2005**.
- **Junior Research Fellowship**, Indian Institute of Science, Bangalore, **2000 – 2002**.

☉ PROFESSIONAL HONORS, ACHIEVEMENTS & SERVICES

- **Fellow of Royal Society of Chemistry (FRSC), London, UK, 2020.**
- **Member of the Editorial Board** of Journal of Molecular Structure, **2022 – 2025.**
- Member of UC Berkeley's Executive Leadership Academy (ELA) Alumni, **2021**.
- **Member of the Advisory Board** of *CrystEngComm* –Journal by Royal Society of Chemistry, **2021**
- **Editor** of Current Indian Science: Crystallography, to be launched by Bentham Science **2021**
- **Member** of the Commission on Quantum Crystallography (QCr) of the IUCr, **2021 – 2024.**
- **Consultant** to the Commission on Quantum Crystallography (QCr) of the IUCr, **2020 – 2021.**
- **Member of National Committee** for International Union of Crystallography (IUCr), **2020 – 2023.**
- **Chairperson** for the Sagamore XX conference of the IUCr Commission of QCr **2024.**
- **Core committee member** at the Shiv Nadar University for **Institution of Eminence, 2020**
- **Panelist** for evaluating the **startup** applicants from **Venture Challenge 4.0** supported by AIM NITI Aayog, GoI, HCL, Dassault Systemes, and HeadStart, **2021**.
- Ph.D. Thesis **reviewer and examiner, IACS, Kolkata and Warsaw University, Poland, 2021.**
- **Adjudicative reviewer** for *ChemComm* **2020**.
- **Regional coordinator** of Kishore Vaigyanik Protsahan Yojana (**KVPY**) – **2020** interview for Delhi -2 centre at Shiv Nadar University.
- **Emerging Investigators** in *Crystal Growth & Design* – An ACS journal, **2019.**
- **Associate Editor** of MOJ Bioorganic & Organic Chemistry published by MedCrave **2017**.
- **National Program Committee member** of Indian Crystallographic Association, **2016**.
- **Session Chair** at the 46th National Seminar on Crystallography (NSC46), 27-29 June 2018, Bengaluru, India.
- **Session Chair** and **judge** for the poster session at the 44th National Seminar on Crystallography (NSC44), July 10-13, **2016**, Pune.
- Program **committee member** of 44th National Seminar of Crystallographic Meeting, **2016**.
- **Reviewer** of Science and Engineering Research Board (SERB), Govt. of India, **2016 - 2021**.
- **Reviewer** of Information Technology Research Academy project proposal, Govt. of India, **2015**.
- **Science Reviewer** of neutron diffraction ANSTO facility, Sydney, AUSTRALIA, **2015-2016**.
- Featured in “**Faculty in Spotlight**” of Shiv Nadar University **2015**.
- **Judge** for the poster sessions at the 23rd congress and general assembly of the International Union of Crystallography (IUCr **2014**), 5-12 August, Montreal, Quebec, **Canada**.
- **Science Reviewer** of the Oak Ridge National Laboratory's Neutron Sciences Directorate, **2014-20**.

☉ Reviewer of articles in the following Journals

1. *The Journal of American Chemical Society*.
2. *Advanced Functional Materials*, Wiley-VCH.
3. *Chemical Communication*, Royal Society of Chemistry.
4. *Crystal Growth & Design*, American Chemical Society.
5. *The Journal of Physical Chemistry A*, American Chemical Society.
6. *Physical Chemistry Chemical Physics*, Royal Society of Chemistry.
7. *CrystEngComm*, Royal Society of Chemistry.
8. *Journal of Molecular Structure*, Elsevier.
9. *Inorganic Frontiers*, Royal Society of Chemistry.
10. *ACS Omega*, American Chemical Society.
11. *Acta Crystallographica Section B*, International Union of Crystallography.
12. *Acta Crystallographica Section C*, International Union of Crystallography.
13. *Journal of Applied Crystallography*, International Union of Crystallography.
14. *Journal of Biomolecular Structure & Dynamics*, Taylor & Francis.
15. *Journal of Chemical Sciences*, Springer.

☉ PROFESSIONAL MEMBERSHIP

- Fellow of Royal Society of Chemistry (FRSC), London, UK
- Member of UC Berkeley's Executive Leadership Academy (ELA) Alumni, 2021.
- Member of the Editorial Board of *Journal of Molecular Structure* – Elsevier, 2022 – 2025.
- Member of the Advisory Board of *CrystEngComm* –Royal Society of Chemistry, 2021
- Editor of Current Indian Science: Crystallography, to be launched by Bentham Science
- Member of the Commission on Quantum Crystallography (QCr) of the IUCr
- Consultant to the Commission on Quantum Crystallography (QCr) of the IUCr
- Member of National Committee for International Union of Crystallography (IUCr), 2020 – 2023
- Associate Editor of MOJ Bioorganic & Organic Chemistry published by MedCrave
- Member of National Program Committee of Indian Crystallography Association
- Member of Indian Institute of Science Alumni Association
- Member of Indian Crystallography Association
- Member of Marie-Curie Alumni Association

☉ CONFERENCE AND MEETINGS

Oral Presentations

1. **(Invited Speaker)** at the 48th National Seminar on Crystallography, IIT **Roorkee**, 25-27 November 2021.
2. **(Invited Speaker)** at the Global SCXRD Users Meeting (Virtual), **Asia**, 11 - 12 November, **2021**.

3. **(Invited Speaker)** at the Second Discussion (Virtual) Meeting on Quantum Crystallography: expectations and reality, **Italy**, 9 – 12 September **2021**.
4. **(Invited Speaker)** at the International Webinar Series on Current Trends in Condensed Matter Physics at Department of Physics, **Goa University**, on 29th September – 1st October **2020**.
5. **(Invited Speaker)** at the Bruker Single Crystal X-ray Diffraction and user Training at IIT **Kanpur**, 27 - 28 February **2020**.
6. **(Invited Speaker)** at the Solid State and Structural Chemistry Unit (SSCU) alumni symposium, Indian Institute of Science, **Bengaluru**, 13th December, **2019**.
7. **(Invited Speaker)** at the National Conference on Advanced Functional Materials-2019 (NCAFM-2019), **New Delhi**, November 20-21, **2019**.
8. **(Invited Speaker, did not attend)** at the Asian Crystallographic Association (AsCA2019), **Singapore**, 17 – 20 December **2019**.
9. **(Invited Speaker)** at the 1st International conference on Crystal Engineering: From Molecules to Crystals, **Raipur**, India, 30 - 31 March **2019**.
10. **(Invited Speaker)** at the International Union of Crystallography (IUCr)'s Sagamore XIX Conference on Quantum Crystallography, Halifax, **Canada**, 8-13 July **2018**.
11. **(Invited Speaker)** at the 46th National Seminar on Crystallography (NSC46), Bengaluru, **India**, 27-29 June **2018**.
12. **(Invited Speaker)** at the 24th Congress & General Assembly of the International Union of Crystallography 2017, **Hyderabad**, 21 – 28 August **2017**.
13. **(Invited Speaker)** at the 1st South East Asia Conference on Crystal Engineering (SEACCE), Colombo, **Sri Lanka**, September 5-7, **2016**.
14. **(Invited Speaker)** at the 44th National Seminar on Crystallography (NSC44), **Pune**, July 10-13, **2016**.
15. **(Invited Speaker)** One day Prof. R. C. Paul national symposium at the Chemistry Department, 23rd, Panjab University, **Chandigarh**, January **2016**.
16. **(Invited Speaker)** at the National symposium on “X-ray diffraction and Recent Advances in Crystallography (XDRAC2015)”, Periyar University, **Salem**, February 27 -28, **2015**.
17. **(Invited Speaker)** at the 8th USPEX workshop on Crystal Structure Prediction, Shiv Nadar University, Dadri, UP, January 20 -24, **2015**.
18. **(Invited Speaker)** at the 3rd China-India-Singapore (CIS) conference on Crystal Engineering, IISc. **Bangalore**, December 7-10, **2014**.
19. **(Invited Speaker)** at the First International Conference on Emerging Materials: Characterization & Application (EMCA-2014), **Kolkata**, December 4-6, **2014**.
20. The 23rd congress and general assembly of the International Union of Crystallography (IUCr), Montreal, Quebec, **Canada**, 5-12 August, **2014**.
21. **(Invited speaker)** National Seminar on Crystallography, IISER-**Mohali**, **2014**.
22. **(Invited speaker)** National Seminar on Crystallography, **New Delhi**, **2013**.
23. **(Invited speaker)** Synchrotron Charge Density School, APS, **Chicago**, IL, USA, **2013**.
24. American Crystallographic Association meeting, **New Orleans**, LA, USA, **2011**.

25. Gordon Research Conference on Electron Distribution & Chemical Bonding, **Mount holyoke college, MA, USA, 2010.**
26. Congress and General Assembly of the IUCr, **Osaka, Japan, 2008.**
27. (**Invited speaker**) National seminar on Crystallography, **Kolkata, 2008.**
28. Sagamore meeting, **Warwickshire, UK, 2006.**

Poster Presentations:

1. At the 48th National Seminar on Crystallography, IIT **Roorkee**, 25-27 November **2021.**
2. At the 25th Congress & General Assembly of the International Union of Crystallography, 12 – 14 August **2021** in Prague (**3 posters**).
3. At the Quantum Crystallography Online Meeting (QCrOM2020), 26th – 29th August 2020 (**3 posters**), **France.**
4. At the 46th National Seminar on Crystallography (NSC46), 27-29 June **2018**, Bengaluru, India.
5. The 24th Congress & General Assembly of the International Union of Crystallography, 21 – 28 August **2017** in Hyderabad (**3 posters** with my students and collaborator).
6. The 44th National Seminar on Crystallography (NSC44), Indian Institute for Science Education and Research (IISER), Pune during July 10-13, **2016 (2 posters).**
7. The 13th Asian Conference of the Asian Crystallographic Association, 05 – 08 Dec **2015**, Kolkata. (**2 posters**)
8. One-Day National Symposium on “Current Trends in Drug Discovery Research in India” Shiv Nadar University, UP, India, **2015. (2 posters)**
9. National Symposium on Opportunities & Challenges in Condensed Matter & Material Physics, Shiv Nadar University, UP, India, **2014.**
10. National Seminar on Crystallography, Indian Institute for Science Education and Research (IISER), Mohali, India, **2014.**
11. American Crystallographic Association, New Orleans, LA, USA, **2011**, Boston, MA, USA, **2012.**
12. Annual Young Investigators' Meeting, Boston, MA, USA, **2010.**
13. European Crystallographic Meeting, Istanbul, Turkey, **2009.**
14. Congress and General Assembly of the International Union of Crystallography, Osaka, Japan, **2008.**
15. ANSTO – AINSE Neutron School on Materials, Sydney, NSW, Australia, **2008.**
16. Gordon Research Conference on Electron Distribution & Chemical Bonding, MA, USA, **2004, 07.**
17. School of Modelling in Solid State Chemistry, London, UK, **2004.**
18. Congress and General Assembly of the IUCr. Geneva, Switzerland, **2002.**
19. Asian Crystallographic Association, Bangalore, India, **2001.**
20. National seminar on Crystallography, Mumbai, India, **2001.**

- **CONFERENCE, WORKSHOPS AND SCHOOLS MANAGED**

- American Chemical Society funded Chemistry Fair **2022** (Moto: Learning by doing) at the Chemistry Department, Shiv Nadar University.
- Sagamore XX conference of the IUCr Commission of QCr, to be held in India in **2024**.
- *Open House cum Science Fair* at Shiv Nadar University in November **2015, 2016, 2017** and **2018**.
- *Asian Charge Density workshop*, Indian Institute of Science, Bangalore, February 23rd – 26th, **2015**.
- *Smart APEX X-ray diffraction user workshop* at IISc., Bangalore, April **2004**
- *Workshop on structural biology*, ORNL, USA, May **2011**, June **2012** and June **2013**.
- *National school on neutron and X-ray scattering*, ORNL, USA, June **2011** and August **2012**.

SELECTED WORKSHOPS ATTENDED

- *Faculty Development Workshop* at the SNU, UP, India, Jan **2015**, Jul **2015**, Jan **2016** and Jan **2017**.
- *8th USPEX workshop on Crystal Structure Prediction*, SNU, Dadri, UP, Jan 20 -24, **2015**.
- *SNU-Duke Faculty Development Workshop* at the Shiv Nadar University, UP, India, July **2014**.
- “*What Can You Do With Neutrons?* May 19-20, **2011**, Oak Ridge National Laboratory, TN, USA.
- School of Modelling in Solid State Chemistry, London, UK, **2004**.

LECTURES DELIVERED AS SEMINARS: 20

1. Shiv Nadar University, Dadri, UP, **2013, 2014, 2015, 2016, 2017, 2018, 2019, India**
2. Indian Institute of Science Education Research, Pune, **2016, India**
3. Punjab University, Chandigarh, **2016, India**
4. Indian Institute of Science Education Research, Mohali, **2013, India**
5. North Bengal University, **2013, India**
6. Oak Ridge National Laboratory, **2010, 2011** and **2013, USA**.
7. Central University of Hyderabad, **2010**, Hyderabad, **India**.
8. University of Henri Poincare, Nancy, **2009, France**.
9. University of Warsaw, Warsaw, **2009, Poland**.
10. National Chemical Laboratory, **2008**, India.
11. Indian Institute of Science, **2001, 2003, 2004, 2008** and **2019**, Bangalore, **India**.
12. University of Durham, Durham, **2004, UK**.

- **Ph.D. STUDENTS' ACHIEVEMENTS (SELECTED)**

Dr. Kunal Kumar Jha:

- Postdoctoral Fellowship at the Faculty of Chemistry, University of Warsaw, Poland December 2018 - present.
- Oral presentation at the 24th Congress and General Assembly of the International Union of Crystallography (IUCr 2017), 21 - 28 August 2017. Hyderabad, India.
- Bursary award to attend the IUCr 2017, Hyderabad, India.

- Oral presentation at the Royal Society of Chemistry Workshop, 15 December, 2016, Shiv Nadar University, Dadri.
- Bursary award to attend National Seminar on Crystallography (NSC44), July'16, IISER Pune, India.
- Recipient of best poster award in one-day symposium, 11 April 2015, Shiv Nadar University, India.
- Bursary award to attend Asian Charge Density workshop, 23-26 Feb 2015, IISc. Bangalore, India.
- Bursary award to attend IUCr Mathcryst and CIMS workshop, 27-31 October 2014, IIT BHU.

Dr. Suman Kumar Mandal:

- Postdoctoral Research Associate, Bristol BioDesign Institute, School of Chemistry/School of Biochemistry, University of Bristol, UK, March 2021 – present.
- Technical Officer for Single-crystal X-ray diffraction and DSC-TGA facilities at SNU, Sept 2020 – Feb 2021.
- Selected for the 52nd Course (Quantum Crystallography) of International School of Crystallography, 1st to 10th June, 2018, Erice, Italy.
- International Travel Support (ITS) from SERB, India Govt. to attend International School of Crystallography, 1st to 10th June, 2018, Erice, Italy.
- Oral presentation at the 24th Congress and General Assembly of the International Union of Crystallography (IUCr 2017), 21 - 28 August 2017, Hyderabad, India.
- Bursary award to attend the IUCr 2017, Hyderabad, India.
- Bursary awarded to attend NSC44, 10th to 13th, July 2016, IISER Pune, India.
- Oral presentation in the New Instruments and Methods session of International Symposium on Diffraction Structural Biology 2016 at the Oak Ridge National Laboratory (ORNL) Knoxville, TN, USA (could not attend).
- Oral presentation at the 13th Conference of Asian Crystallographic Association (AsCA) 5th to 8th, December 2015, Kolkata, India.
- Bursary awarded to attend the 13th Conference of AsCA, 5th to 8th, December 2015, Kolkata, India.
- Bursary awarded to attend Asian Charge Density workshop, 23-26 Feb'15, IISc. Bangalore, India.

Dr. Sanjay Dutta:

- Postdoctoral Research Associate, Department of Chemistry and Biochemistry, Baylor University, Waco, TX, Joining February 2022.
- Bursary award to attend the 25th Congress and General Assembly of IUCr (Virtual), August 14- 22, 2021, Prague.
- Senior Research Fellow, Chemistry Department, Shiv Nadar University, July 2021 – present.
- Awarded with the direct CSIR-SRF in the materials science category, October 2020.
- "IUCr Young Scientists Award" for attending the 16th Conference of the Asian Crystallographic Association (AsCA2019) 17 – 20 December 2019, Singapore.
- Oral Presentation by Sanjay Dutta at the 16th Conference of AsCA2019, 17 – 20 December 2019, Singapore.
- Winner of the best poster presentation award in the NSC46, Bengaluru 27 - 29th June 2018.
- Received Bursary award to attend the MSSC2017 - Ab initio modelling in Solid State Chemistry, in Imperial College London, UK, during September 2017.
- International Travel Support from SERB-DST, India Govt. 2017.

- Bursary award to attend the 24th Congress and General Assembly of IUCr, August 21-28, 2017, Hyderabad, India.

Mr. Anil Kumar:

- Postdoctoral Fellowship at the Faculty of Chemistry, University of Warsaw, Poland. To join in July 2022.
- Oral presentation at the 48th National Seminar on Crystallography, IIT Roorkee, 25-27 November 2021.
- Bursary award to attend the 25th Congress and General Assembly of IUCr (Virtual), August 14- 22, 2021, Prague.
- Poster presentation at the 25th Congress and General Assembly of IUCr (Virtual), August 14- 22, 2021, Prague.