Curriculum Vitae

Dr. Venkatesha R. Hathwar
Assistant Professor and Programme Director of Physics
School of Physical and Applied Sciences,
Goa University,
Taleigao Plateau, Goa - 403 206.
Co-editor: Journal of Applied Crystallography, IUCr
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Education

Ph. D. in Crystallography (2011)
Indian Institute of Science (IISc), Bangalore, India
Mentor: Prof. T. N. Guru Row

M. Sc. in Physics
Mangalore University, Karnataka, India

Research Interest and Expertize

X-ray and Neutron diffraction, Single crystal and Powder diffraction, Rietveld refinement, Synchrotron radiation, Quantum Crystallography, Computational methods, *Insitu*-cryocrystallography, Electron density analysis, High Pressure, Phase transitions, Luminescent materials, Hybrid functional materials, Photocatalysis, Crystal Engineering, Polymorphism, Structural Materials Science

Employment and Research Experience

UGC - Assistant Professor: Goa University, India (October 2018 – Present)

Assistant Professor: University of Tsukuba, Japan (May 2016 - September 2018)

Post Doctoral Fellow: Aarhus University, Denmark (May 2013 - April 2016)

Mentor: Prof. Bo B. Iversen

Post Doctoral Fellow: University of Augsburg, Germany (April 2012 - March 2013)

Mentor: Prof. Wolfgang Scherer

Administrative Experience

Programme Director of Physics at School of Physical and Applied Sciences, Goa University (Jan 2024 – Present)

Member of Board of Studies in MSc Mathematics, Goa University (Nov 2024 – Oct 2027)

Member of Board of Studies in MSc Physics, Goa University (Oct 2024 – Sept 2027)

Member of Management Committee for Materials Characterization Laboratory (MCL) at Goa University (Feb 2024 – Jan 2027)

Member of DST-PURSE project implementation Committee at Goa University (Dec 2023 – Nov 2027)

Member of Board of Studies in MSc Electronics, Goa University (May 2022 – April 2025)

Member of Library Committee at Goa University (August 2021 – July 2024)

Powder XRD Instrument in-charge, Goa University (Aug 2021 – Present)

Awards and Recognitions

- **Co-Editor of the Journal of Applied Crystallography**, International Union of Crystallography (IUCr) Journals, England (Nov 2024 – present).
- **UGC-Faculty Recharge Programme** selected faculty- Cycle IV, UGC, India
- **AsCA Rising Star Award** at The Joint Conference of the Asian Crystallographic Association (AsCA) and Chinese Crystallographic Society held at Beijing, China, 2009.
- **Travel Grant Award** of $1000 by Asian Crystallographic Association (AsCA) to attend AsCA conference at Beijing, China, 2009.
- **Nature Publishing Group GRC Award,** Nature Publishing group, New York, USA, April 2010.
- **Oral presentation prize** at 39th National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, 2010.
- **Poster presentation prize** at Unit day of Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India, 2010.
- **Summer Research Fellowship** from JNCASR, Bangalore, India in 2002.
- **Summer Research Fellowship** from Indian Academy of Sciences, Bangalore India in 2001

Research Grants received as PI

Funding Agency: UGC
Project Title: Synthesis, Characterization and Optical Properties of Charge-Transfer Cocrystals
Duration: 2019-2022 (Completed)
Amount: 10 Lakhs

Funding Agency: UGC-DAE-CSR
Project Title: Correlation of Structural and Multiferroic Switching in Photoluminescent Organic-inorganic Hybrid A2MCl4 Perovskites: Effect of Organic and Transition Metal Cations on the Switching Mechanism
Duration: 2022-2025 (Ongoing)
Amount: 12.35 Lakhs

Teaching and Courses Development (~ 8 years)

Bridge Course in Mathematical Methods

Mathematical methods of physics

Introduction to Crystallography and X-ray Diffraction

Solid State Physics

Solid State Physics Practical

Supervision Experience

PhD Students

1. Mahendra Choudhary
   Topic: Study of structure-property correlations in rare-earth based photoluminescent materials (Since: June 2021)

2. Irshad Ahamad Shaikh
   Topic: Investigation of all inorganic and organic-inorganic hybrid perovskites for photoluminescent applications (Since: June 2021)

Chapters in Book

1. Sunil, S., Nayak, S. K., **Hathwar, V. R.**, Chopra, D., Row, T. N. G. 'Role of Fluorine in Weak Interactions in Co-crystals'. In: **Pharmaceutical Salts and Co-crystals**, Eds. Wouters, J. and Quere, L. Publisher: Royal Society of Chemistry, London, 2011.

2. **Hathwar, V. R.** 'Experimental charge density analysis in organic solids'. In: Understanding intermolecular interactions in the solid state- Approaches and techniques, Ed: Deepak Chopra, Publisher: Royal Society of Chemistry, London, 2018.

Review Articles

1. **Hathwar, V. R.** 'Validation of chemical bonding by charge-density descriptors: The current scenario' *J. Indian Inst. Sci.* 2017, 97, 281-298.
2. Thomas, S.P.; Dikundwar, A.G.; Sarkar, S.; Pavan, M.S.; Pal, R.; **Hathwar**, **V.R**.; Row, T.N. G. 'The relevance of experimental charge density analysis in unraveling noncovalent interactions in molecular crystals' Molecules, 2022, 27, 3690.

Journal Publications

1. Choudhary, M. B.; Jhonson, D.; Das, D. K.; Thiruvenkatam, V.; Kundu, J.; **Hathwar, V. R**. 'Effect of synthesis methods, biocompatibility and photoluminescence of scheelite type sodium lanthanide double tungstates'
   Sci. Rep. 2025, 15, Accepted (DOI:10.1038/s41598-025-93239-3)

2. Jakhi, S. J.; Dhanetwal, M.; Reddy, V. R.; **Hathwar, V. R**.
   'The effect of transition metal on structure and order-disorder phase transition in layered hybrid metal halides $(CH_3CH_2NH_3)_2MCl_4$ (M = Mn and Co)'
   Acta Cryst. Sect. B 2025, 81 (Accpted).

3. Kudlu, A.; Sarma, D.; Das, D. K.; Shamla, A. B.; Bakthavatsalam, R.; **Hathwar, V. R**.; Mahata, A.; Kundu, J.
   'Unravelling the structure–luminescence relationship in two dimensional antimony(III)-doped cadmium(II) halide hybrids'
   J. Mater. Chem. C 2025, 13, 808-820.

4. Singh, S.; Marayathungal, J. H.; Das, D. K.; Khan, A. A.; Bakthavatsalam, R.; **Hathwar, V. R**.; Kundu, J.
   'Rational Design of Zero-dimensional Manganese(II) Halide Hybridswith Suppressed

Melting Temperatures'
J. Phys. Chem. C 2024, 128, 14849-14859.

5. Sharma, S.; Jacob, N.; Grandhi, G. K.; Choudhary, M. B.; Ippili, S.; **Hathwar, V. R.**; Vivo, P.; Lo, R.; Motapothula, M.; Jayaramulu, K.
'Synergistic metal halide perovskite@metal-organic framework hybrids for photocatalytic CO_2 reduction'
iScience 2024, 27, 110924.

6. Sahoo, B. R.; **Hathwar, V. R.**; Deshpande, U. P.; Bhobe, P. A.
'Local structural distortions and thermochromic properties of $Cs_2NaFeCl_6$ halide double perovskite'
J. Mater. Chem. A 2024, 12, 33699-33706.

7. Vernekar, B. K.; Kotkar, G. D.; D'souza, L. R.; **Hathwar, V. R.**; Dhuri, S. N.
'Crystal structure, biological and docking studies of solvothermally isolated novel schiff base'
J. Mol. Stru. 2024, 1295, 136537.

8. Anilkumar, G. N.; **Hathwar, V. R.**
'Quantifying weak interactions in ferroelectric and paraelectric phases of phenazine and chloroanilic acid co-crystal using experimental and theoretical electron densities'
Acta Cryst. Sect. B 2023, 79, 450-461.

9. Das, D.; Bakthavatsalam,R.; **Hathwar,V.R**.; Pallepogu, R.; Kundu, J.
'Intrinsic vs. extrinsic STE emission enhancement in ns sup(2) ion doped metal (Cd, In) halide hybrids'
J. Mater. Chem. C 2023, 11, 3855-3864.

10. Marayathungal,J.H.; Das,D.K.; Bakthavatsalam,R.; Sam,J.; **Hathwar**, **V.R**.; Pallepogu, R.; Dutta, S.; Kundu, J.
'Mn^{2+}-Activated Zero-Dimensional Metal (Cd, Zn) Halide Hybrids with Near-Unity PLQY and Zero Thermal Quenching'
J. Phys. Chem. C 2023, 127, 8618-8630.

11. Kudlu,A.; Das, D.K.; Bakthavatsalam, R.; Sam, J.; Ray, R.; Mondal, M.; Dutta,D.; **Hathwar**, **V.R**.; Pallepogu,R.; Kundu, J.
'Strong Dopant–Dopant Electronic Coupling in Emissive Codoped Two Dimensional Metal Halide Hybrid'
J. Phys. Chem. Lett. 2023, 14, 4933-4940.

12. Arora, V.; Yasmin,E.; Tanwar, N.; **Hathwar**, **V. R**.; Wagh, T.; Dhole, S.; Akshai Kumar
'Pincer-ruthenium-catalyzed reforming of methanol-selective high-yield production of formic acid and hydrogen'
ACS Catal. 2023, 13, 3605-3617.

13. Acharya,P.; Kuila,A.; Pramanik, U.; **Hathwar**, **V.R**.; Brandao,P.; Mukherjee, S.; Maity, S.; Maity, T.; Maity, R.; Samanta, B.C.
'Combined theoretical and experimental insights on DNA and BSA binding interactions of Cu(II) and Ni(II) complexes along with the DPPH method of antioxidant assay and cytotoxicity studies'
RSC Adv. 2023, 13, 7632-7644

14. Mandal, K.; Hasija, A.; Shukla,R.; **Hathwar**, **V.R**.; Chopra, D.
'Quantitative evaluation of the electronic features involving "nucleophilic–electrophilic" character in the chalcogen sulfur'
Phys. Chem. Chem. Phys. 2023, 25, 19427-19434.

15. Mandal, K.; Sarkar, S.; Ghosh, P.; **Hathwar**, **V.R**.; Chopra, D.
'Quantitative insights into noncovalent interactions involving halogen and tetrel bonds in 2,4,6-trimethylpyrylium tetrafluoroborate'
Acta Cryst. Sect. C 2023, 78, 597-605.

16. Thomas, S.P.; Dikundwar, A.G.; Sarkar, S.; Pavan, M.S.; Pal, R.; **Hathwar**, **V.R**.; Row, T.N. G.
'The relevance of experimental charge density analysis in unraveling noncovalent interactions in molecular crystals'
Molecules 2022, 27, 3690.

17. Anilkumar, G. N.; **Hathwar, V. R.**
'Quantitative investigation of halogen and hydrogen bonding in 2-chloro, 4-X-benzoic acids'
Chemistry Select 2022, 7, e202104338.

18. Santhoshkumar, B., Rao, P. L., Ramanathan, K. V., Bera, A. K., Yusuf, S. M., **Hathwar, V. R**., Pahari, B.
'Structure and ionic conductivity of Na3+*x*Sc2Si*x*P3-*x*O12 (*x*=0.0, 0.2, 0.4, 0.8) NASICON materials: A combined neutron diffraction, MAS NMR and impedance study'
Solid State Sci*.* 2021, 111, 106470

19. **Hathwar**, **V.R**.; Bhowal, R.; Chopra, D.
"Insights from electron density analysis into the charge transfer mechanism in a photoluminescent cocrystal of phenanthrene and tetrafluoro-1,4-benzoquinone"
J. Mol. Stru. 2020, 1208, 127864.

20. Bhargao, P.H.; **Hathwar**, **V.R**.; Srinivasan, B.R.
'A Zinc(II) coordination polymer based on a chain of $\{Zn_2O_7\}$ bitetrahedra bridged by 3-methoxybenzoates'
Chemistry Select 2020, 5, 9820-9824.

21. Shi, M. W.; Thomas, S. P.; **Hathwar, V. R**.; Edwards, A. J.; Piltz, R. O.; Jayatilaka, D.; Koutsantonis, G. A.; Overgaard, J.; Nishibori, E.; Iversen, B. B.; Spackman, M. A.

'Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Host−Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis'
J. Am. Chem. Soc. 2019, 141, 3965−3976.

22. **Hathwar, V. R**.; Nakamura, A.; Kasai, H.; Suekuni, K.; Tanaka, H. I.; Takabatake, T.; Iversen, B. B.; Nishibori, E.
'Low-Tempertue structural phase transitions in thermoelectric tetrahedrite $Cu_{12}Sb_4S_{13}$ and tennantite, $Cu_{12}As_4S_{13}$'
Cryst. Growth. Des. 2019, 19, 3979-3988.

23. Kasai, H.; Tolborg, K.; Sist, M.; Zhang, J.; **Hathwar, V. R**.; Filsø, M. Ø.; Cenedese, S.; Sugimoto, K.; Overgaard, J.; Nishibori, E.; Iversen, B. B.
'X-ray electron density investigation of chemical bonding in van der Waals materials'
Nat. Mater. 2018, 17, 249-252.

24. Fugel, M.; Jayatilaka, D.; Hupf, E.; Overgaard, J.; **Hathwar, V. R.**; Macchi, P.; Turner, M. J.; Howard, J. A. K.; Dolomanov, O. V.; Puschmann, H.; Iversen, B. B.; Burgi, H; Grabowsky, S. Probing the accuracy and precision of Hirshfeld atom refinement with HARt interfaced with Olex2
IUCrJ 2018, 5, 32-44.

25. Sirohiwal, A., **Hathwar, V. R.**, Dey, D., Chopra, D.
'Investigation of Chemical Bonding in In Situ Cryocrystallized Organometallic Liquids'
***ChemPhysChem* 2017**, 18, 2859 – 2863.

26. **Hathwar, V. R.**, Stingaciu, M., Richter. B.,Overgaard, J., Iversen, B.
'Variable-temperature structural studies on valence tautomerism in cobalt bis(dioxolene) molecular complexes'
***Acta Crystallogr. Sect. B* 2017**, 73, 304-312.

27. Jørgensen, M. R. V., Piccoli, P. M. B., **Hathwar, V. R.**, Wang, X., Hoffmann, C. M., Yakovenko, A. A., Halder, G. J., Schlueter, J. A., Iversen, B. B., Schultz, A.J.
'Neutron and X-ray investigations of the Jahn–Teller switch in partially deuterated ammonium copper tutton salt, $(NH_4)_2[Cu(H_2O)_6](SO_4)_2$ Jahn–Teller switch'
***Acta Cryst. Sect. B* 2017**, 73, 87-93. Impact Factor: 2.89

28. Sirohiwal, A., **Hathwar, V. R.**, Dey, D., Regunathan, R., Chopra, D.
'Characterization of fluorine-centered 'F···O' σ-hole interactions in the solid-state'
***Acta Crystallogr. Sect. B* 2017**, 73, 140-152.

29. **Hathwar, V. R.**, Thomsen, M. K., Mamakhel, A. H., Filso, M. O., Overgaard, J., Iversen, B.
'Electron Density Analysis of the "O−O" Charge-Shift Bonding in Rubrene Endoperoxide'

***J. Phys. Chem. A* 2016**, 120, 7510−7518.

30. Dey, D., Bhandary, S., Sirohiwal, A., **Hathwar, V. R.**, Chopra, D.
'Conformational lock via unusual intramolecular C–F···O=C and C–H···Cl–C parallel dipoles observed in in situ cryocrystallized liquids'
***Chem. Commun.* 2016**, 52, 7225-7228.

31. **Hathwar, V. R.**, Sist, M., Jørgensen, M. R. V., Mamakhel, A. H., Wang, X., Hoffman, C., Sugimoto, K., Overgaard, J., Iversen, B.
'Quantitative Analysis of Intermolecular Interactions in Orthorhombic Rubrene'
***IUCrJ* 2015**, *2*, 563-574.

32. **Hathwar, V. R.**, Chopra, D., Panini, P., Row, T. N. G.
'Revealing the polarizability of organic fluorine in the trifluoromethyl group: Implications in supramolecular chemistry'
***Cryst. Growth Des.* 2014**, *14*, 5366−5369.

33. Overgaard, J., Walsh, J. P. S., **Hathwar, V. R.**, Jørgensen, M. R. V., Hoffman, C., Platts, J. A., Piltz, R., Winpenny, R. E. P.
'Relationships between electron density and magnetic properties in water-bridged dimetal complexes'
***Inorg. Chem.* 2014**, 53, 11531-11539.

34. Jørgensen, M. R. V., **Hathwar, V. R.**, Bindzus, N., Wahlberg, N., Chen, Y., Overgaard, J., Iversen, B.
'Contemporary X-ray electron density studies using synchrotron radiation'
***IUCrJ* 2014**, 1, 267-280.

35. Jørgensen, M. R. V., **Hathwar, V. R.**, Sist, M., Wang, X., Hoffman, C., Briseno, A. L., Overgaard, J., Iversen, B. B.
'Accurate atomic displacement parameters from time of flight neutron diffraction data at TOPAZ'
***Acta Cryst. Sect. A* 2014**, 70, 679-681.

36. Gnanasekaran, R., **Hathwar, V. R.**, Kumaradhas, P.
'Intermolecular interactions, charge density distribution and the electrostatic properties of pyrazinamide anti-TB drug molecule: an experimental and theoretical charge density study'
***Acta Cryst. Sect. B* 2014**, *70*, 568-379.

37. Gnanasekaran, R., **Hathwar, V. R.**, Kumaradhas, P.
'Topological analysis of electron density and the electrostatic properties of isoniazid: an experimental and theoretical study'
***Acta Crystr. Sect. B* 2014**, *70*, 331-341. Impact Factor: 2.89

38. Lahtinen, M., Kudva, J., Hegde, P., Bhat, K., Kolehmainen, E., Nonappa, **Hathwar, V. R.**,

Naral, D.
'Synthesis, Characterization, Thermal and Antimicrobial studies of *N*-substituted Sulfanilamide derivatives'
***J. Mol. Struc.* 2014**, *1060*, 280-290.

39. Scheidt, E.-W., **Hathwar, V. R.**, Schmitz, D., Dunbar, A., Scherer, W., Tsurkan, V., Deisenhofer, J., Loidl, A.
'Superconductivity at T_c=44 K in $Li_xFe_2Se_2(NH_3)_y$'
***Eur. Phys. J. B.* 2012**, *85*, 279.

40. Arputharaj, D. S., **Hathwar, V. R.**, Row, T. N. G., Kumaradhas, P.
'Topological Electron Density Analysis and Electrostatic Properties of Aspirin: An Experimental and Theoretical Study'
***Cryst. Growth Des.* 2012**, *12*, 4357−1366 (**Coverpage article**).

41. Ganapayya, B., Jayarama, A., Sankolli, R., **Hathwar, V. R.**, Dharmaprakash, S. M.
'Synthesis, growth, and characterization of a new NLO material 3-(2,3-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one'
***J. Mol. Struc.* 2012**, *1007*, 175−178.

42. **Hathwar, V. R.**, Paul, A. K., Natarajan, S., Row, T. N. G.
'Charge density analysis of a pentaborate ion in an ammonium borate: Towards the understanding of topological features in borate minerals'
***J. Phys. Chem. A* 2011**, *115*, 12818−12825.

43. **Hathwar, V. R.**, Thakur, T. S., Dubey, R., Pavan, M. S., Row, T. N. G., Desiraju, G. R.
'Extending the supramolecular synthon based fragment approach (SBFA) for transferability of multipole charge density parameters to monofluorobenzoic acids and their co-crystals with isonicotinamide: importance of C–H···O, C–H···F and F···F intermolecular regions'
***J. Phys. Chem. A* 2011**, *115*, 12852−12863.

44. **Hathwar, V. R.**, Row, T. N. G.
'Charge density analysis of hetero–halogen (Cl···F) and homo–halogen (F···F) intermolecular interactions in molecular crystals: Importance of the extent of polarizability'
***Cryst. Growth Des.* 2011**, *11*, 1338−1346.

45. **Hathwar, V. R.**, Gonnade, R. G., Munshi, P., Bhadbhade, M. M., Row, T. N. G.
'Halogen bonding in 2,5-dichloro-1,4-benzoquinone: Insights from experimental and theoretical charge density analysis'
***Cryst. Growth Des.* 2011**, *11*, 1855–1862.

46. **Hathwar, V. R.**, Thakur, T. S., Row, T. N. G., Desiraju, G. R. 'Transferability of multipole charge density parameters for supramolecular synthons: A new tool for quantitative crystal engineering'
***Cryst. Growth Des.* 2011**, *11*, 616–623.

47. **Hathwar, V. R.**, Row, T. N. G.
'Nature of Cl···Cl intermolecular interactions *via* experimental and theoretical charge density analysis: Correlation of polar flattening effects with geometry'
***J. Phys. Chem. A* 2010**, *114*, 13434–13441.

48. **Hathwar, V. R.**, Pal, R., Row, T. N. G.
'Charge density analysis of crystals of nicotinamide with salicylic acid and oxalic acid: An insight into salt to co-crystal continuum'
***Cryst. Growth Des.* 2010**, *10*, 3306–3310.

49. **Hathwar, V. R.**, Roopan, S., Subashini, R., Khan, F., Row, T. N. G.
'Analysis of Cl···Cl and C–H···Cl intermolecular interactions involving chlorine in substituted 2-chloroquinoline derivatives'
***J. Chem. Sci.* 2010**, *122*, 677–685.

50. Munshi, P., Jelsch, C., **Hathwar, V.R.**, Row, T. N. G.
'Experimental and theoretical charge density analysis of polymorphic structures: The case of coumarin 314 dye'
***Cryst. Growth Des.* 2010**, *10*, 1516–1526.

51. Manivel, P., Khan, F. N., **Hathwar, V. R.**
'Synthesis of diversified thioethers, 1-aroylalkylisoquinolin-1-yl thioethers by electrophilic s-alkylation of 3-phenylisoquinoline-1(2H)-thione'
***Phosphorus, Sulfur and Silicon* 2010**, *185*, 1932–1942.

52. **Hathwar, V. R.**, Manivel, P., Khan, F. N., Row, T. N. G.
'Evaluation of intermolecular interactions in thiocoumarin derivatives: The role of sulfur atom in generating packing motifs'
***CrystEngComm* 2009**, *11*, 284–291.

53. **Hathwar, V. R.**, Prabakaran, K., Subashini, Manivel, P., Khan, F. N.
'3-Phenyl-1-[2-(3-phenylisoquinolin-1-yl)-diselanyl]isoquinoline'
***Acta Cryst. Sect. E* 2008**, *64*, o2295.

54. **Hathwar, V. R.**, Manivel, P., Khan, F. N., Row, T. N. G.
'3–Butyl–1H–isochromen-1-one'
***Acta Cryst. Sect. E* 2007**, *63*, o3707.

55. **Hathwar, V. R.**, Manivel, P., Khan, F. N., Row, T. N. G.
'3–Butyl–1H–isochromen-1-thione'
***Acta Cryst. Sect. E* 2007**, *63*, o3708.

Professional Training Received

Refresher Course in Natural Sciences
UGC-HRDC, Goa University, 15-28 September, 2020

Refresher Course in Experimental Physics

Department of Physics, Goa University, Goa, 12-27 November, 2018

Asian Charge Density Workshop
Indian Institute of Science, Bangalore, 23-26 February, 2015

International School on Charge Density- Theory and Practice
Universidad de Zaragoza, Jaca, Spain, 30th August to 4th September 2011

Workshop on *Ab Initio* Modelling in Solid State Chemistry
Imperial College London, London, UK, 13-17 September 2010.

Indo-Italian Workshop on Application of Synchrotron Radiation to Condensed Matter Problems: Basic and applied research
Indian Institute of Science, Bangalore, 23-25 November 2009

Workshop on XD2006 program package, Advanced Methods in X- Ray Charge Density Analysis: Extracting Properties from a Multipole Refinement
Martina Franca, Italy, 3-6 September 2007.

Workshop on X-Ray Diffraction Methods for Pharma Industry
Indian Institute of Science, Bangalore, India, 2006.

Membership

Life member of Indian Crystallographic Association

Editorial Board Member for Current Indian Science: Crystallography by Bentham Science

Member of Indian Institute of Science Alumni Association

Conferences and Meetings

Oral Presentations:

1. Role of weak interactions on the structural phase transition in functional materials **Oral presentation**. Sagamore XX conference of Quantum Crystallography. Shiv Nadar Institute of Eminence, Delhi NCR, India 10-15, November 2024.
2. Quantifying Weak Interactions on the Structural and Ferroelectric Phase Transitions in Phenazine and Chloroanilic Acid Cocrystal **Invited Talk.** *50th National Seminar on Crystallography.* CSIR-IMTECH, Chandigarh, India 22-24 Nov 2023.
3. The Structure-Property Correlations in Functional Materials using Synchrotron X-Ray Diffraction. **Invited Talk.** *National conference on 'Emerging Prospectives of Chemical Science in Biological and Technological Aspects'.* Acharya Institute of Graduate Studies, Bangaluru. 13 Jul 2022.
4. X-Ray Diffraction: From Symmetry and Structure to Applications in Materials Science. **Invited Lecture.** *4th Refresher Course in Material Sciences: Recombinant Memetics.* University of Calicut, Kerala. 15 Dec 2021.
5. Resolving Superlattice Structural Phase Transitions in Thermoelectric Tetrahedrites using Synchrotron Data. **Invited Talk.** *48th National Seminar on Crystallography.* IIT Roorkee. 25-27 Nov 2021.
6. Structure-Property Correlations using X-ray Electron Density Models. **Invited Talk.** *National Symposium on Recent Trends in Condensed Matter Physics and Materials*

Science. Goa University. 12-13 Mar 2020.

7. Reaching the gray areas of PXRD using single crystals and synchrotron x-ray data. **(Invited Talk).** *Goa Physics Research Meet.* IIT, Goa. 25 Jan 2020.
8. Observing atomic interactions using X-rays. **Invited talk.** Dept. of Physics, Parvatibai Chowgule College of Arts and Science, Margao, Goa. 10 Aug 2019.
9. Charge density analysis of materials: Beyond the ball and stick model in Crystallography. **Invited talk.** *Seminar on Recent Trends in Structural Chemistry.* School of Chemistry, Goa University. 16 Feb 2019.
10. Oral presentation on 'Unravelling low-temperature crystal structures of thermoelectric materials, $Cu_{12}Sb_4S_{13}$ and $Cu_{12}As_4S_{13}$' in the annual meeting of the Crystallographic Society of Japan held at Hiroshima November 23-24, 2017.
11. 'Magnetic Bistability in Valence Tautomers: Toward Molecular Switches' **Invited talk** at 4th national conference on condensed matter physics and applications held at Manipal University, India during May 23-24, 2016.
12. "Material Design Inputs from Charge Density Analysis in Organic Semiconductors' **Invited talk** at the XXIII International Congress and General Assembly of IUCr held at Montréal, Canada from August 5 - 12, 2014.
13. Oral presentation on "Topological features of short X···X contacts *via* experimental and theoretical charge density" in 39th National Seminar on Crystallography held at University of Jammu, Jammu Tawi, 2010.
14. 'AsCA Rising Star' Oral cum poster presentations on "Topological features of short Cl···Cl contacts *via* experimental and theoretical charge density" in The Joint Conference of the Asian Crystallographic Association and Chinese Crystallographic Society held at Beijing, China, 2009.

Poster Presentations:

1. Poster presentation on 'Low-Temperature Structural Phase Transitions in Thermoelectric Tetrahedrite, $Cu_{12}Sb_4S_{13}$, and Tennantite, $Cu_{12}As_4S_{13}$: Resolving Super-lattice Structure using Synchrotron Data' in the virtual conference of Interdisciplinary Topics in Materials Science (ITAM-2021) organized by IISc, JNCASR, CeNS, Bangalore during 27-30 July, 2021.
2. Poster presentation on "Relationship between Structure and Property in Organic Semiconductors by an Electron Density Analysis" in the Sagamore XVIII conference, Sardinia, Italy, June 7-12, 2015.
3. Poster presentation on "Supramolecular synthon Based Fragments Approach for a transferability of multipole parameters" in the European Charge Density Meeting-ECDM6 at Strbske Pleso, Slovakia 2012.
4. Poster presentation on "Hetero and Homo-halogen Intermolecular Interactions via charge density analysis" in the XXII International Congress and General Assembly of IUCr at Madrid, Spain, 2011.
5. Poster presentation on "Nature of halogen bonding: Insights from experimental and theoretical charge density analysis" in ICCOSS XX held at Indian Institute of Science, Bangalore, 2011.

Conference/ Workshop Managed	Local Organizing Committee member for SAGAMORE XX, IUCr Commission on Quantum Crystallography to be held at Shiv Nadar University, Delhi, India on 11-16, Nov 2024. Local Organizing Committee member for International Conference Advanced Materials (ICAM) held at Goa University, Goa, India on 20-24, Feb 2023. Local Organizing Committee member for National Conference on Electronic Structure (NCSE) held at Goa University, Goa, India on 14-16, Nov 2022. Local Organizing Committee member for the International Webinar Series on Current Trends in Condensed Matter Physics at Department of Physics, Goa University held on 29 September – 1 October 2020.