

## Curriculum Vitae

### **Dr. Venkatesha R. Hathwar**

UGC-Assistant Professor,  
Department of Physics,  
Goa University,  
Taleigao Plateau, Goa - 403 206.  
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### **Education**

**Ph. D.** in X-ray Crystallography  
Indian Institute of Science, Bangalore  
Under the supervision of Prof. T. N. Guru Row

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

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### **Research Interest**

X-ray Crystallography, Charge density analysis, Neutron and Synchrotron diffraction, Single Crystal and Powder X-ray diffraction, Hydrogen bonds and van der Waals interactions, Crystal Engineering

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### **Work Experience**

1. UGC - Assistant Professor, Goa University, India  
October 2018 to present
2. Assistant Professor, University of Tsukuba, Japan  
May 2016 to September 2018
3. Post Doctoral Fellow, Aarhus University, Denmark.  
May 2013 to April 2016. Supervisor: Prof Bo B. Iversen
4. Post Doctoral Fellow, University of Augsburg, Germany.  
April 2012 to March 2013. Supervisor: Prof Wolfgang Scherer
5. Institute Research Associate, Indian Institute of Science, Bangalore.  
April 2011 to March 2012. Supervisor: Prof T. N. Guru Row

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### **Awards and recognitions**

- **UGC-Faculty Recharge Programme** selected faculty- Cycle IV
  - **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, April 2010.
  - **Oral presentation prize** at 39<sup>th</sup> 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 in 2002.
  - **Summer Research Fellowship** from Indian Academy of Sciences in 2001
  - Secured the **highest mark in first BSc Physics** for Mangalore University, India, 2001.
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## Scholarships/Grants received

- Research Fellowship of Indian Institute of Science, India,
- Travel grant from DST, India for neutron data collection at ANSTO, Australia, 2010.
- Foreign travel grant from DST, India to attend Gordon Research Conference on electron density and chemical bonding at Mount Holyhooke, USA, 2010.
- Foreign travel grant from CSIR, India to attend MSSC2010 workshop at Imperial College, London, 2010.
- S. J. Jindal trust merit scholarships in BSc and MSc.

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## 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.

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## 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.

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## Journal Publications

1. 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.
  2. 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.
  3. Sirohiwal, A., **Hathwar, V. R.**, Dey, D., Chopra, D. 'Investigation of Chemical Bonding in In Situ Cryocrystallized Organometallic Liquids' *ChemPhysChem* 2017, 18, 2859 – 2863.
  4. **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.
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5. 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,  $(\text{NH}_4)_2[\text{Cu}(\text{H}_2\text{O})_6](\text{SO}_4)_2$  Jahn–Teller switch'  
*Acta Crystallogr. Sect. B* **2017**, 73, 87-93. Impact Factor: 2.89
  6. Sirohiwal, A., **Hathwar, V. R.**, Dey, D., Regunathan, R., Chopra, D.  
'Characterization of fluorine-centered 'F...O'  $\sigma$ -hole interactions in the solid-state'  
*Acta Crystallogr. Sect. B* **2017**, 73, 140-152.
  7. **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.
  8. 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.
  9. **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.
  10. **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.
  11. Overgaard, J., Walsh, J. P. S., **Hathwar, V. R.**, Jørgensen, M. R. V., Hoffman, C., Platts, J. A., Piltz, R., Winpenney, R. E. P.  
'Relationships between electron density and magnetic properties in water-bridged dimetal complexes'  
*Inorg. Chem.* **2014**, 53, 11531-11539.
  12. 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.
  13. Jørgensen, M. R. V., **Hathwar, V. R.**, Sist, M., Wang, X., Hoffman,
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- C., Briseno, A. L., Overgaard, J., Iversen, B. B.  
'Accurate atomic displacement parameters from time of flight neutron diffraction data at TOPAZ'  
*Acta Crystallogr. Sect. A* **2014**, *70*, 679-681.
14. 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 Crystallogr. Sect. B* **2014**, *70*, 568-379.
15. Gnanasekaran, R., **Hathwar, V. R.**, Kumaradhas, P.  
'Topological analysis of electron density and the electrostatic properties of isoniazid: an experimental and theoretical study'  
*Acta Crystallogr. Sect. B* **2014**, *70*, 331-341. Impact Factor: 2.89
16. 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. Struct.* **2014**, *1060*, 280-290.
17. 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  $\text{Li}_x\text{Fe}_2\text{Se}_2(\text{NH}_3)_y$ '  
*Eur. Phys. J. B.* **2012**, *85*, 279.
18. 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).
19. Ganapayya, B., Jayarama, A., Sankolli, R., **Hathwar, V. R.**, Dharmaprasanna, 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. Struct.* **2012**, *1007*, 175-178.
20. **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.
21. **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:
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importance of C–H···O, C–H···F and F···F intermolecular regions’  
*J. Phys. Chem. A* **2011**, *115*, 12852–12863.

22. **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.
  23. **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.
  24. **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.
  25. **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.
  26. **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.
  27. **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.
  28. 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.
  29. Manivel, P., Khan, F. N., **Hathwar, V. R.**  
‘Synthesis of diversified thioethers, 1-arylalkylisoquinolin-1-yl thioethers by electrophilic s-alkylation of 3-phenylisoquinoline-1(2H)-thione’  
*Phosphorus, Sulfur and Silicon* **2010**, *185*, 1932–1942.
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30. **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.
31. **Hathwar, V. R.**, Prabakaran, K., Subashini, Manivel, P., Khan, F. N.  
'3-Phenyl-1-[2-(3-phenylisoquinolin-1-yl)-diselanyl]isoquinoline'  
*Acta Crystallogr. Sect. E* **2008**, *64*, o2295.
32. **Hathwar, V. R.**, Manivel, P., Khan, F. N., Row, T. N. G.  
'3-Butyl-1H-isochromen-1-one'  
*Acta Crystallogr. Sect. E* **2007**, *63*, o3707.
33. **Hathwar, V. R.**, Manivel, P., Khan, F. N., Row, T. N. G.  
'3-Butyl-1H-isochromen-1-thione'  
*Acta Crystallogr. Sect. E* **2007**, *63*, o3708.

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**Oral/Poster Presentations  
in Conferences**

1. Oral presentation on 'Unravelling low-temperature crystal structures of thermoelectric materials,  $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$  and  $\text{Cu}_{12}\text{As}_4\text{S}_{13}$ ' in the annual meeting of the Crystallographic Society of Japan held at Hiroshima November 23-24, 2017.
  2. Invited talk on 'Magnetic Bistability in Valence Tautomers: Toward Molecular Switches' at 4th national conference on condensed matter physics and applications held at Manipal University, India during May 23-24, 2016.
  3. 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.
  4. Invited oral presentation on "Material Design Inputs from Charge Density Analysis in Organic Semiconductors" in the XXIII International Congress and General Assembly of IUCr held at Montréal, Canada from August 5 - 12, 2014.
  5. 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.
  6. 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.
  7. 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.
  8. Oral presentation on "Topological features of short  $\text{X}\cdots\text{X}$  contacts *via* experimental and theoretical charge density" in 39<sup>th</sup> National Seminar on Crystallography held at University of Jammu, Jammu Tawi, 2010.
  9. 'AsCA Rising Star' poster cum oral presentations on "Topological features of short  $\text{Cl}\cdots\text{Cl}$  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.
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**Professional Training  
Received**

**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, 30<sup>th</sup> August to 4<sup>th</sup> 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.

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**Membership**

Life member of Indian Crystallographic Association

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