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Designation: Professor

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Educational background:

Ph.D (X-ray Crystallography), Bangalore University, Bangalore, 1997

Post-doctoral Research Fellowships

Post-Doctoral Research at University of Texas, Houston, USA, 2002.
Post-Doctoral Research at University of Toledo, Ohio, USA, 2000-2002.
Post-Doctoral Research at University of Witwatersrand, Johannesburg, SA (Prestigious Fellowship), 1999-2000.
Post-Doctoral Research at Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, 1997-1999.

Teaching interest

Teaching Post-Graduate (Physics) students – Quantum Mechanics, X-ray Crystallography and Molecular Biophysics are the special subjects of my current teaching.

Major research areas:

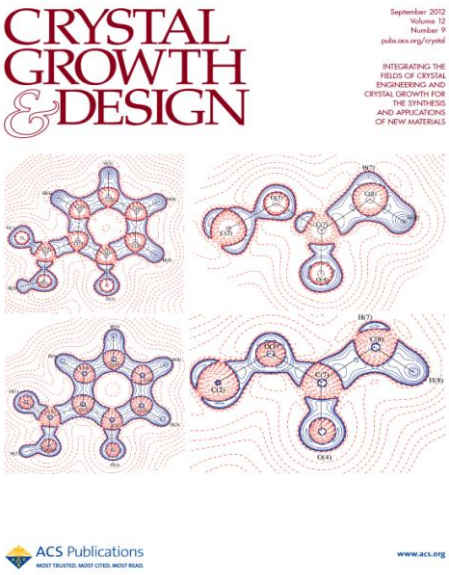
- X-Ray Crystallography (Small and Macromolecules)
- Charge density analysis of molecules via High resolution X-ray diffraction
- Quantum chemical calculations
- Molecular electronics (Nano-devices)
- High energy materials

Current research interests:

- Charge density distribution of high energy materials – Explosives and Propellants - Defense and Space applications.
- Crystal structure prediction of high energetic molecules and Polymorphism in drug molecules.
- Design of molecular Nano-wires, switches and diodes.
- Molecular docking and Molecular modeling -Understanding drug-receptor interactions

- Design of novel drug molecules for TB, Alzheimer and Cancer diseases from plant derived molecules
- X-ray Crystal structure determination of small and macromolecules
- Molecular dynamics (Small and Macromolecules)
- QM/MM Calculation of Ligand-Protein Complexes

Our research articles are in the cover page of Crystal Growth and Design & Acta Cryst. B Journals



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2. Topological electron density analysis and the electrostatic properties of isoniazid: An experimental and theoretical study, Gnanasekaran Rajalakshmi, Venkatesha R. Hathwar and Poomani Kumaradhas, *Acta Cryst. B70, (2014), 331-341.*

List of Research Publications

73. A combined molecular docking and charge density analysis is a new approach for medicinal research to understand drug-receptor interaction: Curcumin-AChE model, A. Renuga Parameswari, G. Rajalakshmi and P. Kumaradhas, *Chemico. Biol. Int.*, (2015), 225, 21-31.

72. Charge density analysis and transport properties of TTF based molecular nanowires- A DFT approach, K. Selvaraju and P. Kumaradhas, *Journal of Nanoscience*, (2014), Press.

71. Charge densiy distribution and electrostatic interactions of ethionamide: an inhibitor of the enoyl acyl carrier protein reductase (inha) enzyme of Mycobacterium tuberculosis, G. Rajalakshmi, Mysore S. Pavan and P. Kumaradhas, *RSC Adv.*, (2014), 4, 57823-57833.

70. Topological electron density analysis and the electrostatic properties of isoniazid: An experimental and theoretical study, Gnanasekaran Rajalakshmi, Venkatesha R. Hathwar and Poomani Kumaradhas, *Acta Cryst. B70, (2014), 331-341*.

69. Intermolecular interactions, charge density distribution and the electrostatic properties of pyrazinamide anti-TB drug molecule: An experimental and theoretical charge density study, Gnanasekaran Rajalakshmi, Venkatesh R. Hathwar and Poomani Kumaradhas. *Acta Cryst. B, (2014),* B70, 568-579.

68. Probing the effect of electric field in 9,10-dimethoxy-2,6-bis(2-*p*-tolylethynyl) anthracene (DMBTA) molecular nanowires using the quantum chemical and charge density analysis. M. Jothi and P. Kumaradhas, *Mol. Simulation*, (2014), 40, 1-10.

67. Ab initio Crystal structure and charge density distribution of High energetic 1,7-Dimethy-1,3,5,7-Tetranitrotrimethylene-Tetramine (OHMX) Molecule: A DFT study P.Srinivasan and P.Kumaradhas, *Proc. HEMCE (2014), 85-93.*

66. Probing the effect of applied electric field in charge density distribution and electrostatic properties of Au substituted saturated polycyclic hydrocarbon molecular nanowires via Quantum chemical and Charge density study. K. Selvaraju, M. Jothi and P. Kumaradhas, *J. Comput. Theor. Nanosci.* (2014), 11, 524-532.

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63. *Ab initio* crystal structure and understanding the bond strength of high energetic 2,4-dinitro benzoic acids molecule via Quantum chemical calculations and charge density analysis, P. Srinivasan, S.N. Asthana, P. Kumaradhas*, *Comb. Explos. and Shock. Waves. (2013), 49, 712-722.*

62. Exploring the effect of External electric field on Octane dithiolate molecular Nanowire: A Quantum chemical and Charge density study. M. Jothi, K. Selvaraju and P. Kumaradhas, *J. Comput. Theor. Nanosci.* (2013), 10, 789-797.

61. Molecular flexibility and the electrostatic properties of curcumin and its derivatives at the active site of p300: A theoretical charge density study, B. Devipriya and P. Kumaradhas*, Chemico. *Biol. Int.* (2013), 204(3), 153-165.

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59. Ab initio crystal structure and understanding the bond strength of high energetic 2,4-dinitro benzoic acids molecule via Quantum chemical calculations and charge density analysis, P. Srinivasan, S. N. Asthana and P. Kumaradhas*, *Comb. Explos. and Shock. Waves. (2013), 49, 712-722.*

58. Bond topological and explosives properties of 2,6-Diamino-3,5-Dinitropyrazine-1-Oxide (LLM-105) energetic molecule, A theoretical study, P. Srinivasan, P. Kumaradhas*, *Conference Proceedings, "New trends research of energetic materials", Czech Republic* (2013), 849-863.

57. Synthesis and structural characterization of organic co-crystals 4,4'-bipyridine-bis(N-phenylanthranilic acid) and 4,4'-bipyridinium-bis(3-carboxypyridine-2-carboxylate), S. Kumaresan, P.G. Seethalakshmi, P. Kumaradhas,* B. Devipriya, *J. Mol. Struct. (2013),* 1032, 169-175

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8. Structural Phase transition in Adipic Acid. Srinivasa Gopalan, R., Kumaradhas, P. and Kulkarni, G. U, *J. Solid State Chemistry, (1999), 148, 129-134.*

7. A charge density study of the polymorphs of p-nitrophenol. Kulkarni. G. U, Kumaradhas, P. and C.N.R. Rao, *Chem. Mat. (1998), 10, 3498-3505.*

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Seminar/ Conference/ Workshops organized

1. Organized National Workshop on "Electrical circuit design and PCB fabrication", Sponsored by UGC, March 27-28, 2012.

2. Organized Special Lectures on "Materials Science", Sponsored by Periyar University, 10th February, 2012.

3. Organized National workshop on "Scientific Application of Powder XRD", Sponsored by Periyar University, 2013.

4. Organized National Seminar on "Scientific usage of Electron Microscopes", Sponsored by Periyar University, 6th January 2014.

5. Organized National Seminar on "Recent Advances in New and Renewable energy", Sponsored by Periyar University, 27th February 2014.

6. Organized Regional "Training Program on Computer Hardware: Assembling and Maintenance", Sponsored by Periyar University, 21-22nd March 2014.

7. Organized Regional "Training Program on Computer Hardware and Networking", Sponsored by Periyar University, 27-28th March 2014.

Research Facilities:

- Single crystal X-ray diffraction with Ultra cooling system
- High Performance Cluster computing facilities to accomplish big scientific computational task in current and future research
- Small and Protein crystal growth facility
- Cold Room crystal growth facility

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