P. A. **Praveen**

Post Doctoral Fellow

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Research

Post Doctoral Fellow — *Jun. 2019 - Present*

Indian Institute of Science Education and Research — *Tirupati, India*

Device fabrication and analysis of OLETs and X-ray sensors

Doctoral Degree — *Jan. 2013 - Jun. 2019*

Bharathidasan University — *Tiruchirappalli, India*

Metal organic nanostructures for thermo-optical applications

Project Student — *Jun. 2010 - Jan. 2013*

Bharathidasan University — *Tiruchirappalli, India*

Improvising organic medium by metal dopants for optical applications

Broad Area of Interest

- **Organic semiconductors** - Synthesis and fabrication of microstructures
- **Photonics** - Device fabrication and measurements
- **Computational materials science** - Modeling structural properties

Education

Post Graduation — *Jul. 2009 - Apr. 2011*

Bharathidasan University — *Tiruchirappalli, India*

First Class with CGPA 7.5

Under Graduation — *Jun. 2006 - Apr. 2009*

Periyar University — *Salem, India*

First Class with 80%

Research

Post Doctoral Work — *Jun. 2019 - Present*

ORGANIC SEMICONDUCTORS FOR OLETs & X-RAY SENSORS

Organic Light Emitting Transistors:

- DFT analysis of biphenylyl end capped oligo-thiophenes with furan substitution
- PVT growth of biphenyly/thiophene derivatives

- Spin coating or thermal evaporation of dielectric layer
- Basic characterizations such as SXRD, PXRD, PL, AFM, SEM
- FET characterization using parametric analyser
- Optical and Electrical pumping of OLETs

Organic X-Ray Sensors:

- PVT growth of pentacene and tetracene systems
- Thermal evaporation for thinfilms
- Basic characterizations such as SXRD, PXRD, PL, AFM, SEM
- Diode characterization using parametric analyser
- Low power X-ray irradiation and corresponding I-V/t sampling

Doctoral Work *Jan. 2013 - Jun. 2019*

METAL ORGANIC THIN FILMS FOR NLO APPLICATIONS

The core objective of the investigation is to analyse the effect of incorporation of metal ions in the benzimidazole (BMZ) medium and to analyse the potentiality of the synthesized system towards NLO applications. There are two strategies, (i) Computational analysis and (ii) Experimental evaluation, were primarily used for the analysis. Primarily, semiempirical quantum chemistry program MOPAC was used for the geometry optimization and molecular properties calculation. Parameters such as bond length, bond angle, dipole moment, energy gap, molecular energy and heat of formation were calculated and used for the interpretation of molecular polarizability and hyperpolarizability values. From the computational analysis three potential candidates Co(II), Cu(II) and Mn(II) were opted for the experimental studies. These metal-BMZ complexes were either deposited as thin films or casted as free standing films depending upon the associated substituent in the metal ion. These samples were subjected to structural and optical characterizations and evaluated for proto-types such as optical limiters (OL) and optical switches (OS). Since, benzimidazole complexes have anticancer activity and found to have a good thermo-optical behavior, they were also investigated for laser assisted anticancer activity.

Important achievements:

- Developed an improved version of chemical solution processing unit
- Physisorption based chemical deposition theory have been successfully developed
- Metal organic thin films of benzimidazole were deposited for the first time
- Home-made Z-scan, OL, OS setups were constructed
- Thermal-assisted anticancer activity with BMZ system was studied for the first time

Awards

2019 **Research Fellowship Award**, Post Doctoral Research, IISER Tirupati, India

2017 **Best Paper Award**, 21^{st} National Seminar on Crystal Growth and Applications, National College, Tiruchirapalli

2016 **Research Fellowship for Meritorious Students in Science**, SRF, UGC, India

2016 **Best Paper Award**, National Conference on Computational and Experimental Physics of Functional Materials, K.S.R College, Tiruchengode

2014 **Third Prize**, DST SERB School on DFT and Beyond, M. S. University, Vadodara

2014 **Research Fellowship for Meritorious Students in Science**, JRF, UGC, India

List of Publications

1. **P. A. Praveen**, A. Bhattacharya, T. Kanagasekaran, A DFT Study on the Electronic and Photophysical Properties of Biphenylyl/Thiophene Derivatives for Organic Light Emitting Transistors, Materials Today Communications 25 (2020) 101509.

2. **P. A. Praveen**, R. Ramesh Babu, Evaluation of nonlinear optical properties from molecular descriptors of benzimidazole metal complexes by principal component analysis, Journal of Molecular Graphics and Modeling 93 (2019) 107447.

3. **P. A. Praveen**, R. Ramesh Babu, P. Balaji, A. Murugadas, M.A. Akbarsha, Laser assisted anticancer activity of benzimidazole based metal organic nanoparticles, Journal of Photochemistry & Photobiology, B: Biology 180 (2018) 218.

4. **P. A. Praveen**, R. Ramesh Babu, K. Ramamurthi, Role of annealing on the structural and optical properties of nanostructured diaceto bis-benzimidazole Mn(II) complex thin films, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 173 (2017) 800.

5. **P. A. Praveen**, R. Ramesh Babu, Theoretical and experimental evaluation of structural and optical properties of novel zinc-benzimidazole metal complex doped in polystyrene matrices, AIP Conference Proceedings 1832 (2017) 140038.

6. **P. A. Praveen**, R. Ramesh Babu, K. Ramamurthi, Theoretical and experimental investigations on linear and nonlinear optical response of metal complexes doped PMMA films, Mater. Res. Express 4 (2017) 025024.

7. **P. A. Praveen**, R Ramesh Babu, Effect of substituents on polarizability and hyperpolarizability values of benzimidazole metal complexes, AIP Conference Proceedings 1731 (2016) 090013.

8. **P. A. Praveen**, R. Ramesh Babu, K. Jothivenkatachalam, K. Ramamurthi, Spectral, morphological, linear and nonlinear optical properties of nanostructured benzimidazole metal complex thin films, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 150 (2015) 280.

9. **P. A. Praveen**, R. Ramesh Babu, K. Ramamurthi, Validation of PM6 and PM7 semiempirical methods on polarizability calculations, AIP Conference Proceedings 1665 (2015) 609.

10. **P. A. Praveen**, S. P. Prabhakaran, R. Ramesh Babu, K. Sethuraman, K. Ramamurthi, Low power optical limiting studies on nanocrystalline benzimidazole thin films prepared by modified liquid phase growth technique, Bulletin of Materials Science 38 (3) (2015) 645.

11. **P. A. Praveen**, R. Ramesh Babu, S. P. Prabhakaran, K. Ramamurthi, Linear and nonlinear optical properties of Mn doped benzimidazole thin films, AIP Conference Proceedings 1591 (1) (2014) 991.

Articles Under Submission

1. **P. A. Praveen**, T. Kanagasekaran, Light Emitting Ambipolar Field Effect Transistors of Biphenylyl-Tetrathiophene Single Crystals with Regio-Specific Emission in Orange Wavelength. *Submitted to ACS Applied Materials & Interfaces*

2. V. Lakshmi Vennila, **P. A. Praveen**, T. Kanagasekaran, N V L Narasimha Murty, Direct X-ray detection using thermally evaporated Pentacene Schottky diodes. *Submitted to Semiconductor Science and Technology: Special Edition on Detectors*

Books

Semiempirical Modeling and Experimental Evaluation of Benzimidazole Based Metal-Organic Complexes for Nonlinear Optical Applications — *Springer*

P. A. Praveen, R. Ramesh Babu — *In Press*

In the book Theoretical Materials Design: Optimization, Simulation and Experimental Realization

Gravitational Waves Explained — *eI Trendz, Tiruchirappalli*

P. A. Praveen — *2018*

Skills

Experimental Techniques

- Thermal Evaporation of metals
- Chemical deposition of thinfilms
- Spin Coating
- PXRD, Raman, FTIR, AFM
- Dielectric, Hall, I-V measurements
- Z-Scan, SHG measurements

Molecular Packages Gaussian, ORCA, MOPAC, AutoDock

Programming Python, Fortran, C++, HTML5, CSS, LaTeX

Academic Activities

Recognized Reviewer — *Elsevier Publications*

Spectrochimica Acta Part A — *Nov. 2018 - Present*

Organizing Committee Member — *Bharathidasan University*

International Conference OnSustainable Energy Technologies — *Jun. 2018*

Organizing Secretary — *Bharathidasan University*

National Science Day Celebrations — *Feb. 2018*

Organizing Committee Member — *Bharathidasan University*

National Science Day Celebrations — *Feb. 2017*

Personal Details

Gender :	Male
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Reference

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Declaration

I hereby declare that all the details furnished above are true to the best of my knowledge and belief.

P. A. Praveen