# P. A. Praveen

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### **Positions**

Postdoctoral Fellow

May. 2023 - Present

Tohoku University, Sendai, Japan.

- Developing furan substituted thiophene co-oligomers for organic lasing
- Using DFT analysis, crystal growth, optical pumping and electrical characterizations

Indian Institute of Science Education and Research, Tirupati, India.

Jan. 2023 – May. 2023

Jun. 2022 - Jan. 2023

- Theoretical analysis of role of furan substitution in pyrene/thiophene systems
- Efficacy of different DFT functionals on predicting optoelectronic properties

Postdoctoral Fellow

University of Tartu, Estonia.

Research Associate

- Design and develop diffractive optical elements for computational imaging
- Performed theoretical and experimental analysis on incoherent holographic systems

Postdoctoral Fellow
 Jun. 2019 – May. 2022

Indian Institute of Science Education and Research, Tirupati, India.

- Design, synthesis and crystal growth of organic semiconductors
- Fabrication of OLETs, low power X-ray sensors and boradband photodetectors

### **Education**

o Doctoral Degree Jan. 2013 – Jun. 2019

Bharathidasan University, Tiruchirappalli

Quantum chemical and experimental analysis of metal organic nanostructures for NLO applications

o Project Student Jun. 2011 – Jan. 2013

Bharathidasan University, Tiruchirappalli

Improvising organic medium by metal dopants for nonlinear optical applications

o Post Graduation Jul. 2009 – Apr. 2011

Bharathidasan University, Tiruchirappalli

First Class (CGPA 7.5)

o Under Graduation Jun. 2006 – Apr. 2009

Periyar University, Salem

First Class (80%)

## **Areas of Expertise**

#### Optoelectronic devices

- Crystal growth and thin film deposition of organic & hybrid perovskite semiconductors
- OFET and organic diodes fabrication and electrical characterization
- Optical pumping, photoluminescence and spectral characteristics of organic semiconductors

#### Metal-organic NLO systems

- Crystal growth / thin film deposition of metal-organic systems
- Nonlinear optical studies SHG and Z-Scan studies

#### Computational materials science

- Materials analysis using DFT and semiemiprical calcualtions
- Excited state dynamics of organic optoelectronic systems

## **Instruments and Packages**

#### Instruments

- Crystal growth: PVT, hydrothermal, low & high temperature solution growth
- Thin films: Thermal evaporation, CVD, spin coating
- Structural: PXRD, Raman, FTIR, SEM/TEM, AFM
- Electrical: Parametric, Dielectric, Hall analyses
- Optical: Optical gain, Indirect imaging, Z-Scan, SHG measurements
- Microfabrication: Laser lablation, photolithography and thermal nano-imprinting

#### Softwares

Gaussian, ORCA, MOPAC, Dalton, AutoDock

Programming

Python, MATLAB, R, FORTRAN

### **Publications**

### Journal Articles

- (22) P. Haldar, **P. A. Praveen**, K. Arulkannan, V. B. Sreegowri and T. Kanagasekaran, "An ultra narrow high quality factor single mode deep blue organic solid state laser", *Optics & Laser Technology*, 2025, **183**, 112379.
- (21) **P. A. Praveen** and T. Kanagasekaran, "Theoretical studies on photophysical properties of luminescent thienylboranes and their suitability towards organic lasing", *Materials Chemistry and Physics*, 2025, **332**, 130268.
- (20) **P. A. Praveen**, T. Kanagasekaran, C. Ma, M. Terada, T. Jin, Y. Wakabayashi and H. Shimotani, "Optoelectronic characteristics of furan substituted thiophene/phenylene co-oligomer single crystals for organic lasing", *Journal of Materials Chemistry C*, 2024, **12**, 15995–16003.
- (19) P. A. Praveen, D. Saravanapriya, S. V. Bhat, K. Arulkannan and T. Kanagasekaran, "Comprehensive analysis of DFT-3C methods with B3LYP and experimental data to model optoelectronic properties of tetracene", Materials Science in Semiconductor Processing, 2024, 173, 108159.
- (18) A. Bhattacharya, **P. A. Praveen**, S. V. Bhat, S. Dhanapal, A. Kandhasamy and T. Kanagasekaran, "Theoretical insights on pyrene end-capped thiophenes/furans and their suitability towards optoelectronic applications", *Computational and Theoretical Chemistry*, 2023, **1225**, 114135.
- (17) A. Bhattacharya, P. A. Praveen and K. Thangavel, "A Combined Theoretical and Experimental Approach to Deduce the Role of Dielectric Layer on Interface Trap Density in Single Crystal Organic Field-Effect Transistors", Crystal Research and Technology, 2023, 58, 2200263.
- (16) A. Bleahu, S. Gopinath, T. Kahro, P. A. Praveen, A. S. J. F. Rajeswary, S. Prabhakar, R. Kumar, G. R. Salla, R. P. Singh, K. Kukli et al., "3D incoherent imaging using an ensemble of sparse self-rotating beams", Optics Express, 2023, 31, 26120–26134.
- (15) A. Jayavel, S. Gopinath, **P. A. Praveen**, F. G. Arockiaraj, A. Bleahu, A. P. I. Xavier, D. Smith, M. Han, I. Slobozhan, S. H. Ng et al., "Improved classification of blurred images with deep-learning networks using lucy-richardson-rosen algorithm", *Photonics*, 2023, **10**, 396.
- (14) S. Gopinath, P. A. Praveen, T. Kahro, A. Bleahu, F. G. Arockiaraj, D. Smith, S. H. Ng, S. Juodkazis, K. Kukli, A. Tamm et al., "Implementation of a large-area diffractive lens using multiple sub-aperture diffractive lenses and computational reconstruction", *Photonics*, 2022, 10, 3.

- (13) M. Han, D. Smith, S. H. Ng, T. Katkus, A. S. John Francis Rajeswary, P. A. Praveen, K. R. Bambery, M. J. Tobin, J. Vongsvivut, S. Juodkazis et al., "Single shot lensless interferenceless phase imaging of biochemical samples using synchrotron near Infrared Beam", Biosensors, 2022, 12, 1073.
- (12) **P. A. Praveen**, F. G. Arockiaraj, S. Gopinath, D. Smith, T. Kahro, S.-M. Valdma, A. Bleahu, S. H. Ng, A. N. K. Reddy, T. Katkus et al., "Deep deconvolution of object information modulated by a refractive lens using Lucy-Richardson-Rosen algorithm", *Photonics*, 2022, **9**, 625.
- (11) **P. A. Praveen**, A. Bleahu, F. Arockiaraj, S. Gopinath, D. Smith, S. Ng, A. Rajeswary, S. Juodkazis and V. Anand, "Digital refocusing of images recorded with white light using Lucy-Richardson-Rosen algorithm", *Asian Journal of Physics*, 2022, **31**, 1027–1034.
- (10) **P. A. Praveen**, P. Muthuraja, P. Gopinath and T. Kanagasekaran, "Impact of furan substitution on the optoelectronic properties of biphenylyl/thiophene derivatives for light-emitting transistors", *The Journal of Physical Chemistry A*, 2022, **126**, 600–607.
- (9) D. Smith, S. Gopinath, F. G. Arockiaraj, A. N. K. Reddy, V. Balasubramani, R. Kumar, N. Dubey, S. H. Ng, T. Katkus, P. A. Praveen et al., "Nonlinear reconstruction of images from patterns generated by deterministic or random optical masks—concepts and review of research", *Journal of Imaging*, 2022, 8, 174.
- (8) V. L. Vineela, **P. A. Praveen**, T. Kanagasekaran, N. Kumar and N. N. Murty, "Direct x-ray detection using thin-film pentacene Schottky diodes", *Journal of Instrumentation*, 2022, **17**, P02024.
- (7) **P. A. Praveen**, A. Bhattacharya and T. Kanagasekaran, "A DFT study on the electronic and photophysical properties of biphenylyl/thiophene derivatives for organic light emitting transistors", *Materials Today Communications*, 2020, **25**, 101509.
- (6) P. A. Praveen and R. R. Babu, "Evaluation of nonlinear optical properties from molecular descriptors of benzimidazole metal complexes by principal component analysis", *Journal of Molecular Graphics and Modelling*, 2019, 93, 107447.
- (5) P. A. Praveen, R. R. Babu, P. Balaji, A. Murugadas and M. Akbarsha, "Laser assisted anticancer activity of benzimidazole based metal organic nanoparticles", *Journal of Photochemistry and Photobiology B: Biology*, 2018, 180, 218–224.
- (4) **P. A. Praveen**, R. R. Babu and 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*, 2017, **173**, 800–808.
- (3) P. A. Praveen, R. R. Babu and K. Ramamurthi, "Theoretical and experimental investigations on linear and nonlinear optical response of metal complexes doped PMMA films", *Materials Research Express*, 2017, 4, 025024.
- (2) **P. A. Praveen**, R. R. Babu, K. Jothivenkatachalam and K. Ramamurthi, "Spectral, morphological, linear and nonlinear optical properties of nanostructured benzimidazole metal complex thin films", *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 2015, **150**, 280–289.
- (1) **P. A. Praveen**, S. Prabhakaran, R. R. Babu, K. Sethuraman and K. Ramamurthi, "Low power optical limiting studies on nanocrystalline benzimidazole thin films prepared by modified liquid phase growth technique", *Bulletin of Materials Science*, 2015, **38**, 645–651.

#### Conference Proceedings

- (12) K. Arulkannan, V. B. Sreegowri, S. Vigneshwaran, **P. A. Praveen**, B. Arka and K. Thangavel, AIP Conference Proceedings, 2025, vol. 3198, p. 020060.
- (11) H. Pratik, D. Saravanapriya, J. Jesmal, **P. A. Praveen** and K. Thangavel, AIP Conference Proceedings, 2025, vol. 3198, p. 020049.
- (10) D. Saravanapriya, H. Pratik, V. B. Sreegowri, K. Arulkannan, **P. A. Praveen** and K. Thangavel, AIP Conference Proceedings, 2025, vol. 3198, p. 020076.

- (9) A. Bleahu, S. Gopinath, R. Kumar, F. G. Arokiaraj, D. Smith, T. Kahro, **P. A. Praveen**, S. H. Ng, A. Pristy, T. Katkus et al., Practical Holography XXXVII: Displays, Materials, and Applications, 2023, vol. 12445, pp. 190–193.
- (8) A. Bleahu, S. Gopinath, A. P. I. Xavier, T. Kahro, A. N. K. Reddy, F. G. Arockiaraj, D. Smith, S. H. Ng, T. Katkus, **P. A. Praveen** et al., Holography: Advances and Modern Trends VIII, 2023, vol. 12574, pp. 153–157.
- (7) S. Gopinath, **P. A. Praveen**, F. G. Arokiaraj, D. Smith, T. Kahro, S.-M. Valdma, A. Bleahu, S. H. Ng, A. N. K. Reddy, T. Katkus et al., Al and Optical Data Sciences IV, 2023, vol. 12438, pp. 329–333.
- (6) S. Gopinath, A. P. I. Xavier, **P. A. Praveen**, T. Kahro, O. Tamm, A. Bleahu, F. G. Arockiaraj, D. Smith, S. H. Ng, S. Juodkazis et al., Holography: Advances and Modern Trends VIII, 2023, vol. 12574, pp. 162–165.
- (5) M. Han, D. Smith, S. H. Ng, T. A. Katkus, A. S. J. F. Rajeswary, P. A. Praveen, M. J. Tobin, J. Vongsvivut, S. Juodkazis and V. Anand, Practical Holography XXXVII: Displays, Materials, and Applications, 2023, vol. 12445, pp. 200–204.
- (4) P. A. Praveen and R. R. Babu, AIP Conference Proceedings, 2017, vol. 1832.
- (3) P. A. Praveen and R. R. Babu, AIP Conference Proceedings, 2016, vol. 1731.
- (2) P. A. Praveen, R. R. Babu and K. Ramamurthi, AIP Conference Proceedings, 2015, vol. 1665.
- (1) **P. A. Praveen**, R. R. Babu, S. Prabhakaran and K. Ramamurthi, AIP Conference Proceedings, 2014, vol. 1591, p. 991.

#### **Book Chapters**

(1) **P. A. Praveen** and T. Kanagasekaran, in *Handbook of Semiconductors: Fundamentals to Emerging Applications*, CRC Press, 2024, p. 81.

## **Funding**

- o Grant-in-Aid for JSPS Fellows (No. 23KF0101) Multiyear funding of ¥2,000,000.
- o Seal of Excellence for MSCA 2024 application.

### **Awards**

- o 2024 IOP Outstanding Reviewer 2023, for the journal Physica Scripta
- 2024 IOP Trusted Reviewer For exceptionally high level peer review competency
- 2023 JSPS Postdoctral Fellowship Post Doctoral Research, Tohoku University, Japan
- o 2022 ERA Chair Postdoctral Fellowship Post Doctoral Research, University of Tartu, Estonia
- 2019 Research Fellowship Award Post Doctoral Research, IISER Tirupati, India
- 2017 Best Paper Award 21<sup>st</sup> 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
- o 2014 Research Fellowship for Meritorious Students in Science JRF, UGC, India

## **Co-Supervision of Graduate Students**

- o 2021 BSMS Vth year Project Fabrication of organic photodetectors for broadband detection
- o 2019 BSMS Vth year Project Effect of different dielectric layers on the mobility of OSCs
- o 2018 M. Sc., Project NLO properties of transistion metal substituted ZIF structures
- 2017 M. Phil., Project Copper based metal organic frameworks for nonlinear optical applications

- 2017 M. Sc., Project Theoretical & experimental analysis of optical properties of cadmium based ZIF structures
- o 2016 M. Sc., Project ZIF-8 thin films for nonlinear optical applications
- 2015 M. Sc., Project Pd doped ZnO nanoparticels for nonlinear optical applications
- o 2014 M. Sc., Project Synthesis of new quinoline derivative for nonlinear optical applications

## **Teaching**

- 2022 Associate Lecturer Graduate Physics Course: Diffractive Optical Elements
- o 2021 Tutor BSMS UG Physics: Mechanics & Optics
- o 2020 Tutor BSMS UG Physics: Mechanics & Optics
- o 2019 Tutor BSMS Advanced Physics: Optics
- o 2019 Tutor BSMS UG Physics: Mechanics & Optics
- o 2018 Tutor M. Sc., (II Year) Materials Science
- o 2017 Tutor M. Sc., (II Year) Materials Science

### **Invited Talks**

- Apr, 2024 Hands-on workshop: Lagar Chennai Institute of Technology, Chennai Beyond the basics: Version control and more
- Jul, 2022 Photonics Summer School, University of Tartu, Estonia
   Organic lasers: concepts, challenges and the story so far
- Jun, 2021 Sri Krishna College of Technology, Coimbatore Roadmap for Research Writing
- Jul, 2020 Jamal Mohamed College (Autonomous), Tiruchirappalli
   Skill Development using Learning Assistance Tools
- Jun, 2020 Jamal Mohamed College (Autonomous), Tiruchirappalli
   Summer School for Online Training on LATEX
- Jun, 2020 Hindustan College of Engineering & Technology, Coimbatore
   Unveiling Molecules: A Computational Materials Science Perspective
- May, 2020 Karpagam College of Engineering, Coimbatore Methods and Tools for Qualitative Research Writing
- Feb, 2018 Dr. SNSR College of Arts & Science, Coimbatore
   One Day Workshop on Lage

#### **Selected Academic Activities**

- Reviewer: Ceramics International, Journal of Physics: Materials, Materials Research Express, Nanotechnology,
   Physica Scripta, Journal of Materials Science: Materials in Electronics, Spectrochimica Acta Part A.
- o Organizing Team Nov. 2022 CIPHR Hackathon, University of Tartu
- Organizing Secretary Feb. 2018 and Feb. 2019 PACE (2018 & 2019), Department of Physics, Bharathidasan University
- o Joint Secretary & Joint Treasurer Jun. 2018 Apr. 2019 Bharathidasan University Physics Forum
- Organizing Committee Jun. 2018 International Conference On Sustainable Energy Technologies, Bharathidasan University
- Organizing Committee Feb. 2014 Seminar on Recent Advances in Materials Science, Bharathidasan University
- Secretray Jul. 2007 Jun. 2008 Physics Club, Department of Physics, K. K. College (Periyar University),
   Namakkal