

## Faculty Profile - Department of Applied Physics



Name: **Dr. A. ABIRAM**

Designation: Assistant Professor

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Area of Specialization: Computational Physics

*Professional Experience: (Total Year of Experience)*

<b>Title of the Profession</b>	<b>Employer</b>	<b>Duration</b>
Assistant Professor	Karunya Institute of Technology and Sciences	9 Years and 2 Months
Post-Doctoral Fellow	University of Lisbon, Portugal	8 Months
Post-Doctoral Fellow	Institute for Drug Research- Hebrew University, Israel	3 Months

Academic Qualification (List from highest to lowest degree)

<b>Degree</b>	<b>Board/University</b>	<b>Year of passing</b>	<b>Class/Grade</b>	<b>Subjects</b>
Doctor of Philosophy in Physics	Bharathiar University	2010	Highly Commended	Computational Physics
Master of Science	Bharathiar University	2004	I <sup>st</sup> Class with Distinction	Physics
Bachelor of Science	Bharathiar University	2002	I <sup>st</sup> Class with Distinction	Physics

Projects Guided

<b>Ph.D</b>			
<b>Name of the Scholar/Student</b>	<b>Title of the Project</b>	<b>Status</b>	<b>Year of Award</b>
Sibin Mon.D.V	Computational study on the modelling of nanocages for adsorption and sensing	Pursuing	--
Abisha Nancy S	Theoretical investigation of metal doped nanoclusters for CO <sub>2</sub> reduction	Pursuing	--
Giftlin George G	Molecular modelling of nanosheets for sensing application.	Pursuing	--
Prince Makarios Paul S	Modelling of nanocages for sensing and adsorption of nerve agents	Pursuing	--
Parimala Devi. D	Dihydrogen bond studies on confine structures	Pursuing	--
<b>M.Sc</b>			
Sibin Mon D. V.	Computational study on the adsorption of A-234 nerve agent on B <sub>12</sub> N <sub>12</sub> nanocluster	Completed	2021
Harini. M	Halogen encapsulation B <sub>12</sub> N <sub>12</sub> of nanocages for magnesium ion battery- A DFT study	Completed	2021
Gokul. G	A theoretical study on the interaction between porphyrin and amino acids	Completed	2019
Prince Makarios Paul S	A theoretical investigation on the interaction of metformin and ferulic acid for antidiabetic activity	Completed	2018
Preeti Tigga	Molecular interaction between Gliclazide and Synephrine for Type 2 Diabetes: A DFT Study	Completed	2018
Giju Tom. G	Effect of hybrid potentials on dihydrogen bonded structure – A theoretical approach	Completed	2017
Abinesh. S	Effects of Catechin on Homocysteine activity – A theoretical approach	Completed	2016

### Details of the Publications

1. Rhodanine-based fluorometric sequential monitoring of silver (I) and iodide ions: Experiment, DFT calculation and multifarious applications, Charles Immanuel David, Gunasekaran Prabakaran, Kaveri Sundaram, Subban Ravi, Duraisamy Parimala devi, **Angamuthu Abiram**, Raju Nandhakumar. *Journal of Hazardous Materials* (**IF: 10.588**) (2021), DOI: 10.1016/j.jhazmat.2021.126449.
2. Theoretical Investigation of Intermolecular Dihydrogen Bonds in C<sub>2</sub>H<sub>2</sub>···HM and C<sub>2</sub>H<sub>4</sub>···HM (M = Li, Na and K) Complexes: A DFT and ab initio Study. D. Parimala devi, Tom Giju, G. Praveena and **A. Abiram**. *Asian Journal of Chemistry*, 33(8) (2021) 0000-0000.
3. Dye sensitized solar cell action of Sn(IV)tetrakis(4-pyridyl) porphyrins as a function of axial ligation and pyridine protonation. Jayachandran, P., **Angamuthu, A.**, Gopalan, P. *Journal of the Iranian Chemical Society* (**IF: 2.019**), 18(7) (2021) 1523–1536.
4. Intermolecular C-H···H-M dihydrogen bonds in five membered heterocyclic complexes - A DFT and ab-initio study, Parimala devi Duraisamy, Praveena Gopalan and **Abiram Angamuthu**. *Monatshefte fur Chemie / (Chemical Monthly)* (**IF: 1.451**), 151(10) (2020) 1569–1579.
5. Effect of peptidic backbone on the nucleic acid dimeric strands, Indumathi, K., **Abiram, A.**, Praveena, G. *Molecular Physics* (**IF: 1.962**) 118(1) (2020) 1-10.
6. Experimental and theoretical studies on a simple S–S-Bridged Dimeric Schiff Base: Selective chromo-fluorogenic chemosensor for nanomolar detection of Fe<sup>2+</sup> & Al<sup>3+</sup> ions and its varied applications, Charles Immanuel David, Nanjan Bhuvanesh, Haritha Jayaraj, Annadurai Thamilselvan, Duraisamy Parimala devi, **Angamuthu Abiram**, Jeyaraj Prabhu, Raju Nandhakumar *ACS Omega* (**IF: 3.512**) 5 (2020)3055-3072.

7. Molecular structure, FT-IR and NMR analyses of dihydrogen-bonded  $B_3N_3H_6 \cdots HM$  complexes: a DFT and MP2 approach, Duraisamy, P., Gopalan, P., **Angamuthu, A.** *Chemical Papers* (**IF: 2.097**) 74 (2020) 1609–1619.
8. TiO<sub>2</sub> Photo Electrode with Gold capping for Improved Observation in Dye Sensitized Solar Cell, Jeba Beula, R., Suganthi, D., **Abiram, A.**, Vidhya, B. *Applied Physics A* (**IF: 2.584**) 126 (2020)1-8.
9. Transforming polymorphs of Co-doped TiO<sub>2</sub> nanoparticles: an efficient photo-electrode for dye-sensitized solar cells, Jeba Beula, R., Suganthi, D., **Abiram, A.**, Vidhya, B. *Applied Nanoscience* (**IF: 3.674**) 10 (2020) 1173–1181.
10. Tris-(2-aminoethyl)amine-intercalated Graphene Oxide as an efficient 2D material for Cerium-Ion fluorescent sensor applications, Elsie, S., Green, A., Rubavathi, D., **Angamuthu, A.**, Gopal, B, Bhagavathsingh, J. *ACS Omega* (**IF: 3.512**) 4 (2019) 22431-22437.
11. Impact of N-(2-aminoethyl) Glycine unit on Watson-Crick base pairs, Karunakaran, I., **Angamuthu, A.**, Gopalan, P. *Zeitschrift fur Physikalische Chemie* (**IF: 2.408**) 233(3) (2019) 449-469.
12. UV-vis absorption spectra of Sn(IV)tetrakis(4-pyridyl) porphyrins on the basis of axial ligation and pyridine protonation, Jayachandran, P., **Angamuthu, A.**, Gopalan, P. *Journal of Molecular Modeling* (**IF: 1.810**) 25(9) (2019) 294.
13. Exploring the structure and stability of  $\beta$ -dipeptide – A quantum chemical and molecular dynamics study, **A. Abiram** and G. Praveena, *Indian Journal of Pure and Applied Physics* (**IF: 0.923**) 56(7) (2018) 561-569.
14. Quantum Chemical Study on the Structure and Energetics of Binary Ionic Porphyrin Complexes, Jayachandran, P., **Angamuthu, A.**, Gopalan, P. *Journal of the Chinese Chemical Society* (**IF: 1.967**) 65(8) (2018) 908-917.

15. Structural and Interaction Properties of Porphyrin Layers – A Quantum Chemical Study, G. Praveena and **A. Abiram**, *Communications in Theoretical Physics* (**IF: 1.968**) 63 (2015) 625.
16. Molecular dynamics and quantum chemical studies on incremental solvation of glycine. A. Yogeswari, R. Kanakaraju, **A. Abiram** and P. Kolandaivel, *Computational and Theoretical Chemistry* (**IF: 1.926**) 967 (2011) 81.
17. Effect of Piratoxin II and Acutohaemolysin Phospholipase (PLA2) proteins on Myristic fatty acid – An ONIOM and DFT study, **A. Abiram** and P. Kolandaivel, *Journal of Molecular Modeling* (**IF: 1.810**) 16 (2010) 1853.
18. Structural analysis and the effect of cyclo(His-Pro) dipeptide on neurotoxins - A dynamics and density functional theory study, **A. Abiram** and P. Kolandaivel, *Journal of Molecular Modeling*, (**IF: 1.810**) 16 (2010) 193.
19. Switching conformation of cyclo (histidyl-histidyl) dipeptide- Dynamics and density functional theory study, **A. Abiram** and P. Kolandaivel, *Molecular Simulation*, (**IF: 2.178**) 35 (2009) 409.
20. Interaction of the tautomeric states of histidine with Cu and Zn metal ions- A theoretical study, **A. Abiram** and P. Kolandaivel, *Journal of Theoretical and Computational Chemistry* (**IF: 0.939**), 8 (2009) 657.
21. Conformational study of palindromic tripeptides (GPG, IPI and KPK) in HIV-1 Protease- A Density Functional theory study, **A. Abiram** and P. Kolandaivel, *Biochimica et Biophysica Acta - Proteins and Proteomics* (**IF: 3.036**), 1774 (2007) 382-391.

Details of the funded projects

<b>Title of the Project</b>	<b>Funding Agency</b>	<b>Duration</b>	<b>Status</b>
A DFT approach towards the coordination of axially ligated Metalloporphyrin on the Au surface - An effective candidate for photodynamic application	SERB - CRG	3 Years	Submitted

Academic and Administrative responsibilities

1. Eduserve co-ordinator for the department
2. Performed as a Co-Coordinator in the Astronomy club
3. Served as Karunya exam coordinator
4. Scrutiny team in admission process
5. Registration committee in single window counselling
6. Regulating committee – Convocation 2015
7. Supported the department in preparing NAAC and UGC files.

Workshop/Symposium/Conference/Seminars organized

1. International webinar series on Astronomy and Astrophysics entitled “*The Sun*” conducted on 28<sup>th</sup> June 2021.
2. International webinar series on Astronomy and Astrophysics entitled “*Are we alone in the Universe*” conducted on 24<sup>th</sup> July 2020.

Invited Talk Delivered

1. Delivered an invited talk on “*Let us know the basics of DFT and its Applications*” in a *two days hands on training programme on computational tools* conducted on 13-14 August 2020 by the Department of Physics, Kalasalingam Academy of Research and Education, Krishnankoil 626 126.
2. Delivered an invited talk on “*Simple S–S-Bridged Dimeric Schiff Bases: A cation targeting Chromo-Fluorogenic Chemosensors*” in the *National Conference on Molecular Modeling and Simulation Methods* conducted by the Department of Physics, PSGR Krishnammal College for Women, Coimbatore on 17<sup>th</sup> and 18<sup>th</sup> February 2020.

3. Delivered an invited talk on “*Nanotechnology-Energizing the Future*” in a seminar conducted by the Department of Physics, SNS College of Technology, Coimbatore on 18<sup>th</sup> March 2016.
4. Delivered an invited talk on “*Let us know Molecular Dynamics*” in a National seminar on Genomics and Proteomics: A Computational Approach conducted by School of Biotechnology, Lady Doak College, Madurai on March 6<sup>th</sup> & 7<sup>th</sup> 2015.

Participation/presentation in Workshop/Seminar/Conference/Symposium/Colloquium

**2020**

- ✓ International Virtual Conference on “High-Performance Materials for Energy, Environment & Healthcare in the Digital Era” - Centre for Materials Technology, School of Advanced Sciences, VIT, Vellore, India.
- ✓ Virtual symposium on “International Day of Light” - Department of Physics, IIT Guwahati.
- ✓ One week faculty development program (FDP) on “Advanced materials research” – Bharat Institute of Engineering and Technology.
- ✓ Online faculty development program (FDP) on “Recent trends in material frontiers” – St. Joseph’s College of Engineering.
- ✓ International Webinar on “Frontiers in Nanotechnology and Applications” - Department of Physics, St.Xavier’s College, Tamilnadu.
- ✓ Webinar on “Wonders of physics - Macro to Nano Technology” – Department of Physics, Medi-Caps University, Indore.

**2019**

- ✓ International conference on sustainable development - Kalasalingam academy of research and education, Krishnankoil, Tamilnadu.
- ✓ Theoretical Chemistry Symposium (TCS) - Birla Institute of Technology and Science, Pilani, Rajasthan.
- ✓ International Conference on Emerging Materials and Modelling - K.S. Rangasamy college of Arts and Science, Tamilnadu

**2018**

- ✓ National Conference on New Energy Materials For Secure and Sustainable Future - S.N. Bose National centre for basic Science, Kolkata and Thiru Kolanjiappar Government Arts College, Tamilnadu.
- ✓ International Conference on Advanced and challenges in chemical sciences - Pachaiyappa's College.
- ✓ International Conference on Advanced Materials for Technological Applications - PSGR Krishnammal College for Women, Coimbatore

### **2017**

- ✓ International symposium on Nanomaterials for Clean Energy and Health Applications - Coimbatore Institute of Technology, Coimbatore.
- ✓ National Conference on Recent Trends in Applied Science and Technology - Alliance College of Engineering and Design

### **2016**

- ✓ National seminar on Strain driven self-assembled semiconductor nanostructures - Karunya Institute of Technology and Sciences, Coimbatore.
- ✓ Participated in a FDP on 'Lecture Capturing' conducted on 23<sup>rd</sup> Aug 2016 at Karunya Institute of Technology and Sciences.
- ✓ Participated in a workshop on virtual lab conducted on 20<sup>th</sup> Feb 2016 by Karunya Institute of Technology and Sciences.
- ✓ Participated in a workshop on Improving effectiveness of teaching and Quality of Education conducted by Karunya Institute of Technology and Sciences on 24<sup>th</sup> June 2016.
- ✓ International Conference on Frontiers in Nanoscience and Nanotechnology - SASTRA University, Thanjavur.
- ✓ National Workshop on Nanomaterials for Energy Applications - Department of Nanotechnology, Anna University, Coimbatore.
- ✓ National Conference on "Modern Materials, Devices and Applications - Maharani's Science College for Women, Bangalore.
- ✓ International workshop on Theoretical and Experimental Physics - Department of Physics, PSG College of Technology, Coimbatore.

### **2015**



- ✓ National seminar on Genomics and Proteomics: A Computational Approach - Madurai Bioinformatics Centre of BTISnet, Lady Doak College, Madurai.

### **2013**

- ✓ Hands on workshop on density functional theory and beyond: Computational material science and real materials - International Centre for Theoretical Physics (ICTP), Italy.
- ✓ International Conference on Innovations in Intelligent and Instrumentation Optimization and Signal Processing - Karunya Institute of Technology and Sciences, Coimbatore, India.

### **2012**

- ✓ Regional Science Congress 2012 - Indian Science Congress Association & Kongunadu Arts and Science College, Coimbatore.
- ✓ National Conference on Nanomaterials - Karunya Institute of Technology and Sciences, Coimbatore, India.

### **2009**

- ✓ International Symposium on - Of Molecules and Materials - Indian Institute of Science Education and Research, Kolkata.

### **2007**

- ✓ School on Biomolecular Simulations - Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India.

### **2006**

- ✓ Theoretical Chemistry Symposium (TCS) - Bharathidasan University, Tamilnadu, India.

### **2004**

- ✓ National conference on recent advances in molecular interactions - PSG College of Arts and Science, Coimbatore, Tamilnadu, India.

### **2003**

- ✓ UGC sponsored seminar on current trend in physics research - Sri Pushpam College, Thanjavur, Tamilnadu, India.
- ✓ State level seminar in holographic imaging and application - Sri Nehru Maha Vidhyalaya (SNMV), Coimbatore, Tamilnadu, India.

### **Other Information**

Guided an intern *Mr. Andreas Beljakov* from Germany on the topic “*Quantum chemistry behind PNA and interaction of PNA with DNA/RNA*” during January 2018- April 2018 under the IAESTE internship program.