



Name : Dr. G. Praveena
Designation : Assistant Professor
Department : Physics
Qualification : Ph. D
Experience : Teaching -14 Years
Research : 17 Years
Area of Specialization(s) : Molecular Quantum Mechanics
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Academic Qualifications

Degree	Brach	Institution/ University name	Year of Graduation
B. Sc	Department of Physics	L.R.G Government Arts and Science College for Women, Tirupur, Tamilnadu, India	Jun 1997- April 2000
M. Sc	Department of Physics	Bharathiar University, Tamilnadu, India.	Jun 2000- April 2002
M. Phil	Molecular Quantum mechanics	Bharathiar University, Tamilnadu, India	Oct 2002- Oct 2004
Ph. D	Molecular Quantum mechanics	Bharathiar University, Tamilnadu, India	Oct 2004- Oct 2009

Research Guidance

Programme	No. of Scholars	
	Completed	Pursuing
Ph. D	3	3

Research Publications (Indexed)

International

1. Rebekah Arulldhas, Praveena Gopalan, Daniel Piecha, Mateusz Szczerba, Exploring the electrocatalytic performance of PdIrSnZnMo high entropy alloy (HEA) towards the hydrogen evolution reaction in an acidic medium: a theoretically supported approach. *Journal of Materials Chemistry A*, 202614(8), 2026.

2. Indumathi Karunakaran, Abiram Angamuthu, Praveena Gopalan, Structure and lowest excitation properties of the backbone-modified GC PNA dimers. *Journal of Chemical Sciences* 137(3),2025.
3. Abisha Nancy Sukumar, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Therapeutic Potential of M@B40 (M = Mg and Ca) Fullerene as a Drug Delivery System for Gemcitabine Anti-Lung Cancer Drug: A DFT Approach. *Chemistry Select* 10(1), 2025.
4. S. Yuvarani, Abiram Angamuthu, **Praveena Gopalan**, A non-catalytic oxidative desulfurization of thiophene and benzothiophene by peroxyacetic acid oxidant. *Theoretical Chemistry Accounts* 143(12) 2024.
5. Abisha Nancy Sukumar, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Investigation of aluminum nitrate nanotube as the smart carriers for targeted delivery of gemcitabine anti-lung cancer drug. *Inorganic Chemistry Communications* 170(3):113309, 2024.
6. Abisha Nancy Sukumar, Parimala Devi, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Pristine B40 fullerene as a potential gemcitabine drug carrier for anti-lung cancer properties: a DFT and QTAIM study. *Journal of Biomolecular Structure and Dynamics*, 44(2):1-14, 2024.
7. Saravanapriya A, Abiram Angamuthu, Praveena Gopalan, DFT study on the electronic and structural properties of M-Salen and M-Salphen electrocatalysts towards effective HER. *Journal of the Indian Chemical Society* 101(11):101381, 2024.
8. Saravanapriya A, Abiram Angamuthu, Praveena Gopalan, Effect of boron halogenation on dihydrogen bonds: A quantum mechanical approach. *Journal of Chemical Sciences* 136(2), 2024.
9. Prince Makarios Paul, Parimala Devi, Abisha Nancy Sukumar, Abiram Angamuthu, Praveena Gopalan, Theoretical insights on the interaction between p-synephrine and Metformin: A DFT, QTAIM and Drug-Likeness investigation. *Computational and Theoretical Chemistry* 1233:114473, 2024.
10. Prince Makarios Paul, Parimala Devi, Praveena Gopalan, Abiram Angamuthu, P. Selvarengan, Impact of Venomous Agent X (VX) Adsorption on the Structural and Electronic Properties of BN Nanosheet, Nanotube and nanocage-A DFT-D3 Study. *Journal of Cluster Science*, 35(5):1-11, 2024.
11. Parimala Devi Duraisamy, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Enhanced hydrogen storage of alkaline earth metal-decorated Bn (n = 3-14) nanoclusters: a DFT study. *Journal of Molecular Modeling* 30(2):55, 2024.
12. Parimala Devi, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Jeba Beula, Investigation of Dihydrogen Bonded Interaction in X₃CH...HNa, X₂CH₂...HNa (X = F, Cl, and Br) Binary and Ternary Complexes: A DFT and DFT-D3 Approach. *Russian Journal of Physical Chemistry* 97(13):3068-3080, 2023.
13. Ranjithkumar Rajamani, Indumathi Karunakaran, Srimathi P, Praveena Gopalan, Abiram Angamuthu, Structure and Reactivity of Halogenated GC PNA Base Pairs – A DFT Approach. *Journal of Experimental Biology and Agricultural Sciences* 11(5):800-808, 2023.
14. Prince Makarios Paul, Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Adsorption behavior of VX nerve agent on X12Y12 nanocages: a density functional theory study. *Structural Chemistry*, 35(4):1-14, 2024.
15. Parimala Devi Duraisamy, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Computational study on alkali and alkaline earth metal decorated B20 cluster for hydrogen storage application. *Structural Chemistry* 35(2):1-10, 2023.

16. Parimala Devi Duraisamy, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Electrochemical properties of endohedral halide (F⁻, Cl⁻ and Br⁻) encapsulated Mg₁₂O₁₂ nanocage for metal-ion batteries. *Inorganic Chemistry Communications*, 157:111359, 2023.
17. Parimala Devi Duraisamy, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Computational study on alkali and alkaline earth metal decorated B₂₀ cluster for hydrogen storage application. *Structural Chemistry*, 35(2):1-10, 2023.
18. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, Electrochemical performance of sodiated 1,4-benzoquinone conformers, *Structural Chemistry*, 34(5), 2023.
19. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, Substitutional effects on the Na-involved electrochemical properties of isomeric benzoquinones, *Computational and Theoretical Chemistry* 1221:114034, 2023.
20. Parimala Devi Duraisamy, Prince Makarios Paul, Praveena Gopalan, Abiram Angamuthu, Feasibility of halide (F⁻, Cl⁻ and Br⁻) encapsulated Be₁₂O₁₂ nanocages as potential anode for metal-ion batteries – A DFT-D3 approach, *Materials Science in Semiconductor Processing* 147:106719, 2022.
21. Parimala Devi Duraisamy, Prince Makarios Paul, Selvarengan Paranthaman, Praveena Gopalan, Abiram Angamuthu, A DFT Study of Halogen (F⁻, Cl⁻, and Br⁻) Encapsulated Ga₁₂X₁₂ (X = N, P, and As) Nanocages for Sodium-Ion Batteries, *Journal of Inorganic and Organometallic Polymers and Materials* 32 (11), 2022.
22. Parimala Devi Duraisamy, Praveena Gopalan, Jeba beula, Abiram Angamuthu, Investigation of dihydrogen bond interaction between Cycloalkenes and alkali metal hydrides: a DFT approach, *Journal of Structural Chemistry* 63 (4):501-509, 2022.
23. Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Investigation of N–H···H–M Dihydrogen Bonded Interactions in Adenine, Cytosine, Guanine, and Thymine with H–M (M = Li and Na) Complexes: A DFT Study, *Russian Journal of Physical Chemistry* 96 (6):1258-1267, 2022.
24. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, Redox potentials of puckered 1,4-benzoquinone, *Journal of Chemical Sciences*, 134 (1), 2022.
25. Prince Makarios Paul, Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Theoretical investigation on the interaction between Metformin and Ferulic acid - A DFT approach, *Journal of the Indian Chemical Society*, 99 (4-5):100368, 2022.
26. A Saravanapriya, G Praveena, Abiram Angamuthu, Molecular Insights on the Dihydrogen Bond Properties of Metal Borohydride Complexes upon Ammoniation, *ECS Journal of Solid State Science and Technology* 10 (9), 2021.
27. Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Theoretical Investigation of Intermolecular Dihydrogen Bonds in C₂H₂···HM and C₂H₄···HM (M = Li, Na and K) Complexes: A DFT and ab initio Study, *Asian Journal of Chemistry*, 33: 1811, (2021).
28. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, Dye sensitized solar cell action of Sn(IV)tetrakis(4-pyridyl) porphyrins as a function of axial ligation and pyridine protonation, *Journal of the Iranian Chemical Society*, 18: 1532-1536, 2021.

29. Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Molecular structure, FT-IR and NMR analyses of dihydrogen-bonded B₃N₃H₆...HM complexes: a DFT and MP2 approach, *Chemical Papers*, 74: 1609-1619, 2020.
30. Parimala Devi Duraisamy, Praveena Gopalan, Abiram Angamuthu, Intermolecular C-H...H-M dihydrogen bonds in five-membered heterocyclic complexes: a DFT and ab-initio study, *Monatshefte für Chemie*, 151: 1569-1579, 2020.
31. Indumathi Karunakaran, Abiram Angamuthu, Praveena Gopalan, Effect of peptidic backbone on the nucleic acid dimeric strands, *Molecular Physics*, 118: 1-10, 2020.
32. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, UV-vis absorption spectra of Sn(IV)tetrakis(4-pyridyl) porphyrins on the basis of axial ligation and pyridine protonation, *Journal of Molecular Modeling*, 25: 294 (1-13), 2019.
33. Sahu, Sumit Ranjan, Parimala Devi. D, Phanikumar.V. V. N., Ramesh, T. Rajalakshmi. N, Praveena G, Prakash. R, Das B, Gopalan, R, Tamarind seed skin-derived fiber-like carbon nanostructures as novel anode material for lithium-ion battery, *Ionics*, 24: 3413-3421, 2018.
34. Abiram Angamuthu, Praveena Gopalan, Exploring the structure and stability of β -dipeptide – A quantum chemical and molecular dynamics study, *Indian Journal of Pure and Applied physics*, 56: 561-569, 2018.
35. Indumathi Karunakaran, Abiram Angamuthu, Praveena Gopalan, Impact of N-(2-aminoethyl) Glycine Unit on Watson-Crick Base Pairs, *Zeitschrift für Physikalische Chemie*, 233: 449-469, 2018.
36. Pavithra Jayachandran, Abiram Angamuthu, Praveena Gopalan, Quantum Chemical Study on the Structure and Energetics of Binary Ionic Porphyrin Complexes, *Journal of the Chinese Chemical Society*, 65: 908-917, 2018.
37. G. Praveena and A. Abiram, A theoretical study of NO, CO and O₂ diatomic molecules interacting between porphyrin layers, *Communications in Theoretical Physics*, 63: 625–634, 2015.
38. S. Neyertz, P. Gopalan, D. Brown, P. Brachet, F. Männle, Oxygen transport in amino-functionalized polyhedral oligomeric silsesquioxanes (POSS), *Soft Materials*, 12, 113-123, 2014.
39. G. Praveena and P. Kolandaivel, Metal ion binding properties of α - γ hybrid cyclic peptide nanotubes – A theoretical study based on the ONIOM method, *IEEE Transaction on NanoBioscience*, 9(2), 100-110, 2010.
40. G. Praveena and P. Kolandaivel, Structural properties and anion binding affinity of cyclo[(1R,3S)- γ -Acc-Gly]₃ hexapeptide, *Journal of Biomolecular Structure and Dynamics*, 27: 37-48, 2009.
41. G. Praveena and P. Kolandaivel, Interaction of metal ions with cyclo[(1R,3S)- γ -Acc-Gly]₃ hexapeptide, *Journal of Molecular Structure - THEOCHEM*, 900: 96-102, 2009.
42. G. Praveena and P. Kolandaivel, Structural and dynamical studies of all-trans and all-cis cyclo[(1R,3S)- γ -Acc-Gly]₃ peptides, *Journal of Molecular Modeling*, 14: 1147-1157, 2008.

43. G. Praveena, P. Kolandaivel, N. Santhanamoorthi, V. Renugopalakrishnan and Seeram Ramakrishna, Looking beyond carbon nanotubes: polypeptide nanotubes as alternatives? *Journal of Nanoscience and Nanotechnology*, 7: 2253-2259, 2007.
44. G. Praveena and P. Kolandaivel, Interaction of Hydrogen Halides and water molecules with the isomers of C20 fullerene – A theoretical Study, *Journal of Molecular Structure*, 828: 154-161, 2007.
45. P. Kolandaivel, G. Praveena and P. Selvarengan, Study of atomic and condensed atomic indices for reactive sites of molecules, *Journal of Chemical Sciences*, 117: 591-598, 2005.

Other Publications: International/National

1. G. Praveena, M. Agalya, K. Nandhini, The interaction of polyethylene with oxygen molecule – A quantum chemical study, *Advances in Applied Research*, 5, 25-31, 2013.
2. J Pavithra, G Praveena, Quantum chemical study on the XH...HM (X= -C2 H, -C2 H3 and M= Li, Na, K, Fe, Zn) dihydrogen bond systems, *Advances in Applied Research*, 10: 1-5, 2018.
3. K Indumathi, G Praveena, Excited states of PNA base pairs – A theoretical approach, *Advances in Applied Research*, 10: 43-46, 2018.
4. J Pavithra, G Praveena, Light absorption properties of binary ionic porphyrin layers in the presence of Cl- axial ligand and pyridine protonation, *Advances in Applied Research*, 11: 93-102, 2019.
5. A Saravanapriya and G. Praveena, Impact of electronegativity on the dihydrogen bond formation in MH...NH complexes, *Advances in Applied Research*, 13 (1):13-17, 2021.

Acted as a Resource Person

1. Invited talk on “Understanding Molecular Diffusion Through Molecular Dynamics” in the National Seminar on Genomics and Proteomics: A Computational Approach, 6 –7, March 2015, Lady Doak College, Madurai, India.
2. Panel Discussion: Effect of COVID-19 on Indian Economy – Policy and Programmatic Implications, May 9, 2020, IIHMR University, Rajasthan, India.
3. DC Committee Member of the Department of Physics,
 1. Karunya Institute of Technology and Sciences, Coimbatore
 2. Bharathiar University, Coimbatore
 3. Government Arts and Science, Coimbatore
4. External Academic Auditor of the Department of Physics, Karunya Institute of Technology and Sciences.
5. AICTE sponsored Faculty Development Program at IFET College of Engineering, 16th November 2017.

Reviewer in journal

- IEEE Access
- Journal of Molecular Modeling
- Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

- Current Computer-Aided Drug Design
- International Journal of Computational and Theoretical Chemistry

Paper Presentations in Conference

International

1. International Workshop on Nanoscience and Nanotechnology, February 13 – 17, 2006, Anna University and International Centre for Theoretical Physics, Trieste, ITALY at Anna University, Chennai, India. Poster presentation: Interaction studies of ring isomer of C₂₀ fullerenes with hydrogen halides, **Awarded: Best poster prize.**
2. “Density Functional Theory and Beyond: Computational Materials Science for Real Materials" Abdus Salam International Centre for Theoretical Physics, August 5-16, 2013. Trieste, Italy. Poster presentation: Metal Ion Binding of the α - γ Hybrid Cyclic Peptide Nanotubes-A Theoretical Study.
3. International Conference on “Frontiers in Nanoscience and Nanotechnology”, February 26-28, 2016, Sastra University, India. Poster presentation: Structure and Energetics of Porphyrin Nanoaggregate

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National

1. School on Biomolecular Simulations, November 6-16, 2007, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) at JNCASR, Bangalore, India. Poster presentation: Structural and dynamical • exploration of all-trans and all-cis cyclo[(1R,3S)- γ -Acc-Gly]₃ peptides.
2. Indian Science Congress, December 15- 16, 2012, Kongunadu arts and science college, Coimbatore, India. Oral presentation: Structural properties of porphyrin layers – A quantum chemical study.
3. Conference on NanoMaterials, December 3-4, 2012, Karunya University, Coimbatore, India. Poster National Conference on “Modern Materials. Devices and Applications”, January 6 - 7, 2016, Sri Maharani College for Women, Bengaluru, India. Poster presentation: Role of Catechin on the Inhibition of Homocysteic Acid Activity.
4. Theoretical Chemistry Symposium, December 11-13, 2006, Bharathidasan University, Tamilnadu, India, Poster presentation: Structural investigation of ligand binding residues of ionotropic glutamate receptor – A molecular dynamics approach.
5. National Conference on NanoMaterials, December 3-4, 2012, Karunya University, Coimbatore, India. Poster Presentation: Interaction of porphyrin layers with diatomic molecules – A theoretical study.

Participation in Conference

- International Conference on Advanced materials for Technological Applications, 3-5 January 2018, PSGR Krishnammal College for Women, Coimbatore.
- International virtual conference on High-performance materials for Energy, Environment & Healthcare in the digital era, Jun 30 - Jul 01, 2022, VIT, Vellore.

- Indo-Taiwan conference on semiconductor packaging & Testing, 30-31 Jan, 2026, SASTRA Deemed University, Thanjavur.

Participation in Workshop

- National Workshop in Molecular Electronic Structure and Dynamics, March 22-24, 2005, Bharathidasan University, Tamilnadu, India.
- Summer School and Workshop on “Electronic Structure Methods and their Applications”, July 10-22, 2006, International Centre for Theoretical Physics, Trieste, ITALY and Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) at JNCASR, Bangalore, India.
- Workshop on High Performance Computing, August 6-9, 2007, Centre for Development of Advanced Computing (C-DAC), Pune and Centre for Non-linear Dynamics, at Bharathidasan University, Tamilnadu, India.
- Two-day workshop on Public Financial Management System (PFMS) with special reference to EAT module, 30th November & 1st December 2018, PSGR Krishnammal College for Women, Coimbatore.
- Workshop on Optics, 16th October 2018, PSGR Krishnammal College for Women, Coimbatore.
- Workshop on Intellectual Property Rights and Management, April 22 – 23, 2016, PSG College for Technology, India.
- CSIR NET/SET Workshop on physical sciences on 12-13 Aug, 2024, PSGR Krishnammal College for Women, Coimbatore.
- CSIR NET/SET Workshop on physical sciences on 14-15 July, 2025, PSGR Krishnammal College for Women, Coimbatore.
- Pre-conference workshop Indo-Taiwan conference on semiconductor packaging & Testing, 29 Jan, 2026, SASTRA Deemed University, Thanjavur.

Conference/Seminar/Workshop Organized

1. Interdisciplinary Students’ Science Conclave: Science for Industry, two-day workshop at PSGRKCW as a convener, Oct 17-18th Feb 2026.
2. Workshop on Integrating AI in Academics and Research, one-day workshop at PSGRKCW as a convener, 28th Aug 2024.
3. Virtual Global Congress on Sustainable Growth & Development 2022-Health and Life sciences as Organizing Secretary on November 25-26, 2022.
4. National Conference on Molecular Modelling and Simulation Methods, two-day workshop at PSGRKCW as a Convener, Feb 17-18, 2020.

Grants

S. No	Project Title	Name of the Agency	Amount	Status
1	Theoretical Investigation of Porphyrin Nanotubes for Photodynamic and Chemical Sensor Applications	Department of Science & technology (DST) SERB-FAST TRACK SCHEME FOR YOUNG SCIENTISTS	5,04,000	Completed
2	Ion Transport Properties of Cyclic Peptide Nanotube – A Theoretical Approach	University Grants Commission (UGC) - Minor Research Project	3,02,061	Completed

Awards/Honors

Awards/Honors	Agency/Institute	Year of Award
Awarded	Best Faculty Award	2022
Awarded	Best Faculty Award	2018
Awarded	Ville de Marseille Scholarship for Post-Doctoral researchers	2010
Awarded	Senior Research Fellowship (SRF)	2006
Awarded	Dr. K. M. Marimuthu Endowment Gold Medal	2002
Awarded	University First Rank	2002
Awarded	University Second Rank	2000
Awarded	National Merit Scholarship	2000

Indexing and Citations

Overall Citation: 366, H- Index = 10.