Arun Kantholi

arunkantholi1@gmail.com — **O** Github

RESEARCH INTERESTS

Computational materials science, Atoms and molecules in strong magnetic fields

COMPUTATIONAL SKILLS

- Programming Languages: Python, MATLAB, LaTeX
- Software/Package: Gaussian, GAMESS, AutoDock Vina, PyMOL, Git/Github, LONDON (quantum chemistry software), Q-Chem (ab initio quantum chemistry software), Orca, Multiwfn, Origin Pro, Quantum Espresso, Office
- **Operating Systems:** Particularly interested in Linux OS, Mac OS, Windows OS. Worked with supercomputers Dirac and as a part of research project at IISER Kolkata for computation with quantum chemistry software.

PUBLICATIONS

Journal paper

1. Impact of Nanosilicon on the Behavior of Polypyrrole Nanocomposites for Gas Sensing Applications

<u>Arun K</u>, Sangita Sen, K. K. Sunisha, S. Sankar, Ramesan, M.T

Journal: Journal of Inorganic and Organometallic Polymers and Materials Link

- 2. Development of High-Performance Polyindole/Silicon Carbide Nanocomposites for Optoelectrical and Sensing Application
 - Gopika.R, <u>Arun K</u>, Ramesan.M.T Journal: ACS Langmuir Link
- In-situ polymerization of polythiophene/silicon carbide nanocomposites for gas sensing and optoelectronic devices Gopika.R, Arun K, Ramesan.M.T

Journal: Journal of Materials Research and Technology Link

- 4. Optimizing the structural, thermal, gas sensing and electrical properties of in-situ polymerized poly(thiophene-co-indole)/silicon carbide nanocomposites for energy storage applications
 Gopika.R, <u>Arun K</u>, Ramesan.M.T
 Journal: Journal of Alloys and Compounds Link
- Nanochitosan Reinforced Polyvinyl Alcohol/Cashew Gum Bio-blend Nanocomposites: Promising Materials for Future Frontiers in Optoelectronic Devices
 Meera, K., <u>Arun K</u>, Ramesan, M.T Journal: Journal of Polymers and the Environment Link
- 6. Effect of Boehmite Nanoparticles on the Properties of Poly (Methyl Methacrylate) Nanocomposites for Flexible Optoelectronic Devices Vyshakh, <u>Arun K</u>, Rohith Sathian, AR Furhan, Meenakshi Verma, MT Ramesan Journal: Journal of Thermoplastic Composite Materials Link
- 7. High-performance Biopolymer Blend Nanocomposites for Flexible Electronic Devices Meera, K., <u>Arun K</u>, Ramesan, M.T *Journal:* Journal of Applied Polymer Science Link
- 8. High-performance poly (ethylene-co-vinyl acetate)/nickel oxide nanocomposite prepared through open mill mixing technique for energy storage applications
 M. Shini, <u>Arun K</u>, Ramesan, M.T *Journal:* Polymer Composites Link

RESEARCH EXPERIENCE

1.Indian Institute Of Science Education And Research Kolkata Visiting Internship Student - Theoretical & Computational Material Science • Exploring Atomic and Molecular Electronic Excitation in Strong Magnetic Fields.

Dr. Sangita Sen Assistant Professor, DCS

2.Indian Institute Of Science Education And Research KolkataKolkata, IndiaJunior Research Fellow - Theoretical & Computational ScienceSept 2022 — Jun 2024

- Exploring Atomic and Molecular Electronic Excitation in Strong Magnetic Fields. Compute excited state magnetic properties of molecules reveals the complex relationship between molecular structure and electronic nature in strong magnetic field
- Relativistic effect in the transition spectra and properties of confined atoms and molecules This research explores how the full relativistic framework influences the behavior of electrons within confined environments, leading to observable changes in the spectral characteristics and overall properties of the studied atomic and molecular systems
- Investigating the singlet-triplet gap values for multi-reference systems. An accurate estimation of the singlet-triplet gap is key to various important chemical phenomena ranging from the designing of solar energy cells to organic light-emitting diodes. To estimate the singlet-triplet gap for multi-reference systems,

Dr. Sangita Sen, Assistant Professor, Department of Chemical Sciences

4. Central University of Tezpur, Assam

Junior Research Fellow-Experimental

- Applied research and development for the industrial realization of lignin recycling and conversion to value-added international market products
- Designing heterogeneous catalysts for the reductive depolymerization of lignin. To efficiently break down lignin into valuable chemical building blocks

Dr. Dhanpati Deka , Professor, Department of Energy

5.	University of Calicut, Kerala, India		Keral	la, 1	India
MS	Thesis Research Project-Experimental	Jan	2020 - C	Oct	2021

• Explored polymer nanocomposites for gas sensing and flexible optoelectronic devices. Incorporated silicon nanoparticles, boehmite nanoparticles, and nanochitosan into polymer matrices to boost performance for future optoelectronic devices and energy storage. The impact of these nanofillers on structural, thermal, electrical, and optical properties was analyzed systematically

Dr. M.T Ramesen, Professor, Department of Chemical Science

6. University of Calicut, Kerala, India		Kerala,	India
BS Thesis Research Project-Experimental	Jan	2013 — Apri	1 2016

• To analyze physical, chemical, and biological parameters of water samples from various sources like wells, ponds, and rivers. Comparative studies were conducted, classifying results based on sample location and source

Dr. Jasila Karayil , Assistant Professor, Department of Chemical Science

SELECTED COURSES

Master's Courses

- Basic concepts in quantum chemistry and group Theory
- Applications of quantum mechanics and group theory
- Molecular spectroscopy
- Electrochemistry, solid state chemistry and Statistical

Bachelor's Courses

- Core Course II Theoretical Chemistry
- 1st Complimentary Course Physics I,II,III
- 2nd Complimentary Course Maths I,II,III
- Core Course III Physical Chemistry I
- Core Course VII Physical Chemistry II

CERTIFICATE COURSE

- NPTEL Online Course : Many body methods in quantum chemistry
- Udemy Online Course: The Complete Python Bootcamp From Zero to Hero in Python. Instructor Jose Portilla
- Coursera Online Course: Supervised Machine Learning: Regression and Classification .

AWARDS

- National Level Graduate Aptitude Test in Engineering in Chemistry conducted by IIT Delhi (90.7 percentile) Mar 2020
- Secured IIT JAM (Joint Admission Test for M.Sc) Chemistry conducted by IIT Bombay Mar 2017

POSTER PRESENTATION & WORKSHOPS

Poster: Computing Excited States properties of molecule under Non-uniform Magnetic Fields: Nonperturbative Approach Inter IISER/NISER Chemistry Meet (IINCM-2024) Click here Kolkata, India Indian Institute of Science Education and Research Kolkata 23th - 24th February 2024
 Poster: Compute Excited State Magnetic Properties of Molecules in Strong Magnetic Field using TDHF - Theoretical Chemistry Symposium (TCS-2023) Madras, India Indian Institute of Technology Madras,India 7th - 10th December 2023
 Virtual Winter School on Computational Chemistry Click here Kolkata 6th-10th February , 2023

EXTRACURRICULAR ACTIVITIES

- NSS volunteer(National Service Scheme, a voluntary program sponsored by the Indian government's Ministry of Youth Affairs and Sports)
- NCC C Certificate holder(National Cadet Corps cadet is a volunteer student who receives basic military training, such as small arms handling and drill exercises, from college)
- I have launched a YouTube channel ; Chemdraw ¿ to communicate chemistry topics
- Hockey, Cricket, football, Gym, etc