Pranay Venkatesh

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chemicalfiend.github.io

Research Interest

I am interested in using theoretical and computational chemical physics tools to model disordered materials and developing the next generation of semiconductor optoelectronic devices.

Education

2019–2024 **M.Sc., Chemistry**, *Birla Institute of Technology and Science*, Pilani, India

2019–2024 **B.E., Chemical Engineering**, *Birla Institute of Technology and Science*, Pilani, India

Research Experience

2023–2024 **Visiting Research Student**, *Frost Group, Imperial College London*, London, England

Mentor: Professor Jarvist Moore Frost at Department of Chemistry, Imperial College London.

- Developed Non-Adiabatic dynamics methods for semiconductor materials to simulate the time-dependent electronic structure of materials under photoexcitation.

summer 2022 **Research Intern**, *Computational Materials Engineering Lab, Boise State University*, Boise, Idaho

Mentor: Professor Eric Jankowski at the Micron School of Materials Science and Engineering, Boise State University at Idaho.

- Analyzed Y6 and BTO materials and assessed their candidacy for organic photovoltaic applications.
- Estimated the force-field parameters of the molecules using MP4 and TD-DFT methods in Gaussian09 as implemented in QUBEKit.
- Determined the morphology and self-assembly of these materials using Molecular Dynamics (MD) simulations in HOOMD-Blue.
- Evaluated the charge-carrier transport properties and electron mobilities using semi-empirical quantum chemical calculations and kinetic monte carlo simulations.
- Presented a poster at ICUR '22 describing our workflow.

2021–2023 **Undergraduate Research Assistant**, *Birla Institute of Technology and Science*, Pilani, India

Mentor : Professor Sarbani Ghosh, Department of Chemical Engineering

- Worked on conducting polymer materials for optoelectronic and gas sensing applications.
- Devised new simulation setups for studying morphology of polymeric systems under nano-confinement.
- Obtained novel results regarding cylindrical nanoconfinement of PEDOT molecules by performing MD simulations in LAMMPS.
- Analyzed the self-assembly patterns of various polymers by writing bespoke computational codes in Julia.

summer 2021 **Summer Intern**, *CSIR - Central Leather Research Institute*, Chennai, India

Analyzed collagen molecules using X-Ray Crystallography and identified key components of its structural biology using the XRD data. Performed multiple sequence alignment studies on ClustalX to identify the patterns in protein sequences that are responsible for causing *Osteogenesis imperfecta* in humans.

Open Source Experience

summer 2022 **Julia Season of Code Contributor**, *JuliaMolSim - Molly.jl*

- Implemented bond and angle constraint algorithms in the Molly.jl framework.
- Coded in analysis features such as velocity autocorrelation.
- Implemented various interatomic potentials and bonded interactions that help model various systems.

Publications

1 Sukanya Das, **Pranay Venkatesh**, Sarbani Ghosh, K S Narayan. Ordered and Disordered Microstructures of Nanoconfined Conducting Polymers, RSC Soft Matter 2023

2 **Pranay Venkatesh**, Eric Jankowski, Gwen White. Computational Challenges to Predicting Morphology of Large Macromolecule Blends, Poster at ICUR 2022

Teaching Experience

spring 2023 **Teaching Assistant**, *Transport Phenomena*

- Wrote comprehensive lecture notes for the course.
- Demonstrated some transport problems and their numerical solutions using simulations.
- Taught a session related to stream function and boundary layer theory in 2D flows.

Projects

fall 2022 **Molecular Dynamics Simulations of Liquids under Ultra-Confinement**, *Study Project, Dept. of Chemistry*, BITS Pilani

Evaluated the properties of nano-scale evaporation of Argon at low temperatures in the presence of a solid with Molecular Dynamics (MD) simulations. Determined the Hamaker coefficient, a metric for "wettability" in an Argon-Platinum system for various geometries.

fall 2022 **Smart Insoles for Shock Absorption**, *Course Project, Introduction to MEMS*, BITS Pilani

Designed an insole with a smart electrorheological gel that works as a shock absorber in athlete's shoes, preventing damage and improving quality of sport. Modelled the gel and the effect of the shoe in COMSOL multiphysics.

fall 2022 **Effective Models for Momentum Transport in Solid-Liquid Interfaces in MEMS Devices**, *Course Project, Transport Phenomena*, BITS Pilani

Obtained velocity profiles for a fluid in a nano-channel under various models. Leveraged direct-simulation monte carlo (DSMC) simulations to determine how slip in a solid-fluid boundary plays a large impact in micro and nano-scale systems.

fall 2022 **Forced Convection Cooling of Integrated Circuits**, *Course Project, Transport Phenomena*, BITS Pilani

Demonstrated the harsh impact of IC heating on a PCB and designed a cooling solution that uses forced convection heat transfer using computational fluid dynamics (CFD) simulations in Ansys Icepak.

spring 2022 **Gallium Nitride Applications and Subsequent Improvements**, *Course Project, Materials Science and Engineering*, BITS Pilani

- Reviewed the use of Gallium Nitride (GaN) in high-speed networks and power electronics. Interviewed prominent researchers in the field to understand the material processing and morphological features of its heterostructure.
- Surveyed diode and transistor device performance with the use of Gallium Nitride composites with NbN and other materials.

spring 2020 **Theoretical Investigation of Aggregation-Induced Emission (AIE) Molecules**, BITS Pilani

Performed TD-DFT calculations with various functionals to reproduce the absorption and emission spectra for a novel Near IR (NIR) emissive molecule.

Technical Experience

Extremely Proficient With

languages Julia, Python

technologies LAMMPS, HOOMD-Blue, LaTeX, Bash Scripting, Git, Vim, Linux, Gnuplot

Have Experience With

languages Fortran-90, Java, Lua, C, MATLAB

technologies VMD, NWChem, Gaussian09, ANSYS Icepak, COMSOL, CUDA, Slurm

Conferences and Workshops

summer 2022 JuliaCon 2022

summer 2022 Idaho Conference on Undergraduate Research

summer 2021 JuliaCon 2021

Relevant Coursework

core courses Materials Science and Engineering, Numerical Methods for Chemical Engineers, Physical Chemistry 2 (Quantum Mechanics), Physical Chemistry 3 (Group Theory and Many-electron Theory), Physical Chemistry 4 (Statistical Mechanics and Theories of Reaction Rates)

electives Electronic Correlation in Atoms and Molecules, Statistical Thermodynamics, Introduction to MEMS, Chemistry of Materials, Transport Phenomena, Quantum Information and Computing

online courses Introduction to Tensorflow, Improving Deep Neural Networks

Extracurriculars and Hobbies

BITS-ACM (Association of Computing Machinery)

Promoted and motivated an understanding of scientific computing within the club. Wrote articles on simple machine learning and game development in python for the BITS-ACM blog.

The Eastern Outlook

Eastern culture and anime club within the institute. Helped conduct events, games, discussions and expositions related to Japanese, Chinese and Korean art forms.

Other Hobbies

Carnatic violin; Cricket; Philosophy; Electronics, operating systems and embedded software