Pranay Venkatesh

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chemicalfiend.github.io

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

Experience

summer 2022 **Research Intern**, *Computational Materials Engineering Lab*, 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.
- Determined the morphology and self-assembly of these materials using Molecular Dynamics (MD) simulations in HOOMD-Blue.
- Identified essential force-field parameters required for simulations using QUBEKit and Gaussian.
- Evaluated the charge-carrier mobilities using quantum chemical calculations and kinetic monte carlo simulations.
- Presented a poster at ICUR '22 describing our workflow.

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.
- Working towards enhancing the visualization and interfacing features of Molly.jl and the JuliaMolSim community.

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.

Projects

present **Electronic Structure, Optical Absorption and Morphology of Conducting Polymers**, *Dept. of Chemical Engg.*, BITS Pilani

- Characterized the optoelectronic properties of PB2T-TEG thin films using TD-DFT simulations in Gaussian.
- Observed the self-assembly of the condensed phase using molecular dynamics (MD) simulations.
- Analysed the charge transport properties using semi-empirical quantum chemical calculations and kinetic monte carlo simulations.

present **Molecular Dynamics Simulations of Liquids under Ultra-Confinement**, *Dept. of Chemistry*, BITS Pilani

Evaluated the flow properties of dense gases in nanochannels using Molecular Dynamics (MD) simulations. Compared simulation results with novel theoretical methods for treatment of two-phase regimes in fluids.

2021–2022 **Substrate Dependent Morphology of Conducting Polymers**, *Dept. of Chemical Engg*, BITS Pilani

Characterized the morphological features and self-assembly of PEDOT:PSS and PEDOT:Tos under a cylindrically constrained alumina frame using Molecular Dynamics (MD) Simulations in LAMMPS. Developed an extensive codebase for the lab to set up, run and analyze simulations.

Technical Experience

Extremely Proficient With

languages Julia, Python

technologies LAMMPS, HOOMD-Blue, Gaussian09, LaTeX, Bash Scripting, Git, Vim, Linux

Have Experience With

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

technologies VMD, NWChem, CUDA, Slurm

Relevant Coursework

core courses Materials Science and Engineering, Numerical Methods for Chemical Engineers, Physical Chemistry 2 and 3 (Quantum Mechanics; Group Theory and Many-electron Theory)

electives Statistical Thermodynamics, Chemistry of Materials, Quantum Information and Computing

online courses Introduction to Tensorflow, Improving Deep Neural Networks