Pranay Venkatesh

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Education

Master of Sciences in Chemistry 2019 - 2024 (expected)
Birla Institute of Technology and Science, Pilani Campus *Third Year Student*

Bachelor of Engineering in Chemical Engineering 2019 - 2024 (expected)
Birla Institute of Technology and Science, Pilani Campus *Third Year Student*

Experience

Summer Research Intern Summer 2022
Computational Materials Engineering Laboratory, Boise State University *Current*

- Identified Y6 and BTO morphology and self-assembly patterns under various conditions to assess their candidacy for photovoltaic devices
- Developed methods for polyellipsoid simulations which assist in running coarse-grained simulations
- Contributed to the lab codebase, in particular towards setting up and preconditioning simulations

Julia Season of Code Summer 2022
JuliaMolSim - Molly.jl *Current*

- Implemented bond and angle constraint algorithms in the Molly.jl framework and working towards enhancing GPU compatibility as part of the Julia Season of Code Programme for 2022.
- Coded in analysis features such as velocity autocorrelation
- Implemented interatomic forces and bonded interactions that help model various systems
- Enhancing the visualization features of Molly.jl and in general the JuliaMolSim community.

Summer Research Intern Summer 2021
CSIR - Central Leather Research Institute *Previous*

- Analyzed collagen using X-Ray Crystallography and identified key components of its structural biology using the XRD data. Performed multiple sequence alignment on ClustalX software to identify sequences responsible for *Osteogenesis imperfecta*.

Projects

Substrate Dependent Morphology of Conducting Polymers Fall 2021 - Present
Study Project, Department of Chemical Engineering *Current*

- Designed an alumina-PEDOT nanocomposite and characterized morphological features under cylindrical constraints using Molecular Dynamics simulations
- Analyzed structural characteristics and phase transitions in conducting polymers using Molecular Dynamics (MD) simulations in LAMMPS
- Developed the codebase for the lab in the Julia programming language, for setting up, running and analyzing simulations

Software Skills

- Programming Languages - Julia, Python, Fortran-90, Java, C, MATLAB, Lua, Haskell
- Software - LAMMPS, HOOMD-Blue, NWChem, VMD, Packmol, Moltemplate, CCP4, Gaussian09, QChem
- Miscellaneous - LaTeX, Bash Scripting, Git, high Linux proficiency

Relevant Coursework

- Core Courses : Materials Science and Engineering, Numerical Methods for Chemical Engineers, Physical Chemistry 2 and 3 (Quantum Mechanics)
- Electives : Statistical Thermodynamics, Chemistry of Materials, Quantum Information and Computing
- Online Courses / MOOCs : Introduction to TensorFlow, Improving Deep Neural Networks (Coursera)