Shubham Sharma

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Education

Indian Institute of Technology Jodhpur — Jodhpur, India
Master of Science in Physics — *June 2019 – June 2021*

- GPA: 8.58/10.00
- Relevant Coursework: Machine Learning, Computational Material Science, Statistical Mechanics, Quantum Mechanics, Soft Matter Physics

Ramjas College, University of Delhi — Delhi, India
Bachelor of Science (Hons.) in Physics — *May 2016 – June 2019*

- GPA: 7.05/10.00 (First Divison)
- Minor in Mathematics

Research Intersts

Machine Learning accelerated Molecular Simulations: applying machine learning techniques with molecular modeling and quantum mechanics to solve fundamental problems in chemical physics

Multiscale Modelling of Soft Matter Physics: development of modeling approaches including the first principle DFT calculations, ab-initio to classical level MD simulations and coarsegrained methods

Experience

Artificial Intelligence Research Intern — June 2021 – Present
CCNSB Lab, IIIT Hyderabad — *Hyderabad, India*

- Working under Dr. Deva Priyakumar (Professor, IIIT Hyderabad) on "Modern Machine learning Applications for Protein-ligand Interactions: Datasets and Algorithms" project
- Building ultra large dataset for Binding affinity prediction for protein-ligand complex interactions

Research Intern — Sep 2019 – June 2021
Computational Physics Lab, IIT Jodhpur — *Jodhpur, India*

- Worked under Dr. Santosh Mogurampelly (Asst. Professor, IIT Jodhpur) on several projects related to Molecular Dynamics Simulations
- Completed my MSc Thesis titled, "Molecular Dynamics Study of Effect of Plasticizers on Ion Transport in Polyethylene Oxide (PEO)-LiTFSI Electrolytes for Li-ion Batteries"

Research Projects

MD Simulation Study of Ion Mechanism in Li-Ion Batteries | *MSc Thesis* — Nov 2020 – June 2021

- Performed molecular dynamics simulations on SPE (i.e. poly(ethylene oxide)) consisting of LiTFSI salt and SN plasticiser
- Calculated the ion diffusivity and explained the ion transport mechanisms
- Illustrated that the mobility of Li^+ and $TFSI^-$ ions is increased upon adding of SN particles
- Found that mobility of $TFSI^-$ ions is completely due to ion-pair interactions whereas for Li^+ ions apart from ion-pair interactions and polymer segmental motion there are other interactions also

Solutions to many-electron Schrödinger equation with deep neural networks — Oct 2020 – Nov 2020

- Used FermiNet- a neural network architecture developed by DeepMind® on DGX-2 (GPU) to calculate ground state energy of LiH, NH_3 and C_2H_4

Molecular Dynamics (MD) Simulations of Argon Gas and Real Water — Mar 2020 – Oct 2020

- Reproduced the equation of state for argon gas and compared it with its real gas behavior
- Simulated the system with water molecules and calculated the RDF, mean-squared displacement and diffusion coeffcient of oxygen-oxygen atoms

Scholastic Achievments

- Secured an All India Rank 487 among 14000 applicants in IIT-JAM 2019
- Scored 95 % in Physics, Chemistry and Mathematics in Senior Secondary Examination, 2016

Additional Information

Programming Languages : Python, C++, MATLAB, JAVA, MySQL, HTML

Theoretical Techniques : MD Simulation, Monte Carlo (MC) Simulation, Density Functional Theory (DFT)

Simulation Packages : GROMACS, LAMMPS, GAUSSIAN, Quantum ESPRESSO, Scikit-Learn, Keras, AMBER

Experienced with performing simulations on High-Performing Clusters (HPCs)

MOOCs – Online Certifications :

- *Neural Networks and Deep Learning offered by DeepLearnong.AI on Coursera.*
- *Specialization on Python for Everybody* offered by University of Michigan on Coursera.
- *Exploring Quantum Mechanics* offered by University of Maryland, College Park on Coursera

Interests : Chess, Cricket and Football