Shubham Sharma

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 $\underline{\mbox{Personal Website}}$ | IIT Jodhpur, Rajasthan, India

Education

Indian Institute of Technology Jodhpur

Master of Science in Physics

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

Ramjas College, University of Delhi

Bachelor of Science (Hons.) in Physics

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

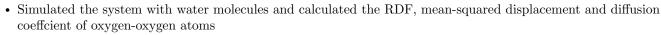
Research Intersts

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	



Jodhpur, India June 2019 – June 2021

May 2016 – June 2019

Delhi, India

- 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