Shubham Sharma

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Education

2019–2021 **Indian Institute of Technology Jodhpur**, *Rajasthan, India*
Master of Science in Physics | CGPA: 8.58/10.00
Thesis: "MD Study of Ion Transport Mechanism in Li-ion Batteries"

2016–2019 **Ramjas College, University of Delhi**, *New Delhi, India*
Bachelor of Science (Hons.) in Physics | CGPA: 7.05/10.00 (First Division)
Minor in Mathematics

Research Interests

Machine Learning for Molecular Simulations
Development and application of ML methods for material design and drug discovery.

Multiscale Modelling of Soft Matter Physics
Development of modeling approaches including the first principle DFT calculations, ab-initio to classical level MD simulations and coarse-grained methods.

Experience

June'21–Present **CCNSB Lab**, *IIIT Hyderabad*
Research Intern (Healthcare) | Advisor: Prof. Deva Priyakumar
- Working on 'Modern Machine Learning Applications for Protein-ligand Interactions: Datasets and Algorithms' project.
- Developed a simulated dataset of 5000 protein-ligand binding affinities for ML-based drug discovery applications.
- Working on chemical retrosynthesis using Transformer based ML model.

Sep'19–June'21 **Computational Physics Lab**, *IIT Jodhpur*
Graduate Student Researcher | Advisor: Prof. Santosh Mogurampelly
- Formulated and worked on several projects related to material design using molecular dynamics simulations.
- Conceived my master's project and wrote thesis titled, 'Molecular Dynamics Study of Effect of Plasticizers on Ion Transport in Polyethylene Oxide (PEO)-LiTFSI Electrolytes for Li-ion Batteries'.
- Explained the 2D Ising Model to entire class by developing a MATLAB code using the Metropolis algorithm [Code].

Publications

Manuscript Under Review

1. **Effect of Succinonitrile on Ion Transport in PEO-based Lithium-Ion Battery Electrolytes** [Paper]
Shubham Sharma, Sipra Mohapatra & Santosh Mogurampelly

2. **PLAS-5k: Dataset of Protein-Ligand Binding Affinities from Molecular Dynamics Simulations** [Website]
Divya B. Korlepara, (and 13 others, including **Shubham Sharma**)

Projects

June'21–Present **Dataset of Protein-Ligand Binding Affinities from Molecular Dynamics Simulations**

- Contributed 1000+ protein-ligand binding affinities using MM-PBSA method.
- Examined the sequence similarities between protein chains using MMseqs2 to show diversity in the dataset.
- Trained OnionNet architecture on PLAS-5k dataset to provide baseline for binding affinity prediction.
- Supervised new interns to acquaint them with the dataset's research methodology and processes.

Nov'20–June'21 **MD Simulation Study of Ion Transport Mechanism in Li-ion Batteries**

- Performed classical molecular dynamics simulations on SPE (i.e. poly(ethylene oxide)) consisting of LiTFSI salt and SN plasticiser.
- Illustrated the enhancing effect of SN particles on mobility of Li and TFSI ions.
- Investigated ion transport mechanisms using ion-pair relaxations and polymer segmental motion of poly(ethylene oxide) chains.

Mar'20–Oct'20 **Molecular Dynamics (MD) Simulations of Argon Gas and Real Water**

- Reproduced the equation of state for argon gas and compared it with the real gas behavior.
- Simulated a TIP3P water model and calculated the RDF, mean-squared displacement, and diffusion coefficient of oxygen-oxygen atoms.

Scholastic Achievements

- **All India Rank 487** among 14000 applicants in IIT-JAM 2019.
- **Scored 95%** in Physics, Chemistry and Mathematics in the Senior Secondary Examination, 2016.
- **Certificate of Merit** for excellence in academics, LPS Ltd, Rohtak, 2017.

Professional Skills

Languages: Advance: Python, MATLAB, Fortran, bash/UNIX scripting | Intermediate: JAVA, LaTeX

Theoretical Techniques: Molecular Dynamics (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).

Additional Information

Aug–Sep'21 Participated in the '5^{th} Summer school on Artificial Intelligence', *CVIT, IIIT Hyderabad* | [Certificates]

Oct'21–Present	Currently enrolled in a year-long certificate program in 'Foundations of Modern Machine Learning' (FMML), *IHub-Data, IIIT Hyderabad*
MOOCs	Neural Networks and Deep Learning, Specialization on Python for Everybody, Understanding Einstein: The Special Theory of Relativity, *Coursera*
Personal Interests	Amateur Chess Player, Football Enthusiast