# Shubham Sharma

+91-7988020138 | sharma.36@iitj.ac.in | B-5/169 IIT Jodhpur, Rajasthan, India

# **EDUCATION**

# Indian Institute of Technology Jodhpur

Jodhpur, India

Master of Science in Physics

Jun 2019 - Present

- GPA: 8.25/10.00 (Till 2<sup>nd</sup> Semester)
- Relevant Coursework: Machine Learning, Computational Material Science, Statistical Mechanics, Quantum Mechanics, Condensed Matter Physics

## Ramjas College, University of Delhi

Delhi, India

May 2016 - Jun 2019

Bachelor of Science (Hons.) in Physics

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

## Research Interests

Physics Based Machine Learning: applying deep learning techniques in the field of computational physics and chemistry

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

# RESEARCH PROJECTS

# Study of the effect of Plasticizers on Ion Transport for Li-ion Batteries

Dec 2020 - Present

• Currently working under **Prof. Santosh Mogurampelly**, as part of MSc. thesis on MD Simulation study of the effect of Lithium Aluminate (LAO) on Ion Transport in Polyethylene Oxide (PEO)-LiTFSI electrolytes for Li-Ion batteries

# Solutions to many–electron Schrödinger equation with deep neural networks

Oct 2020 - Nov 2020

• Used **FermiNet**- a neural network architecture developed by DeepMind<sup>®</sup> on DGX-2 (GPU) to calculate ground state energy of LiH, NH<sub>3</sub> and  $C_2H_4$ 

## Molecular Dynamic (MD) Simulation of Argon | LAMMPS

Aug 2020 - Oct 2020

- Reproduced the equation of state for argon gas
- Compared the result with real gas behaviour of argon gas

### MD Simulation of Real Water | LAMMPS

Nov 2019 - Mar 2020

- Worked with **Prof. Santosh Mogurampelly** to plot the Radial distribution function and mean square displacement of oxygen-oxygen atom
- Calculated the diffusion coefficient of water in the 2fs using Density Functional Theorey (DFT)

## SCHOLASTIC ACHIEVMENTS

- Secured 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 Skills:** Python, MATLAB, C++, JAVA, HTML, MySQL **Technical Skills:** Molecular Dynamics and Monte Carlo Simulations

**Software Packages:** GROMACS, LAMMPS, VMD

# **MOOCs - Online Certifications**

- Completed a Specialization course on Python for Everybody offered by University of Michigan on Coursera
- Completed a course on *Understanding Einstein: Principle of Special Relativity* by Dr. Larry Randles of Stanford University on Coursera

Interests: Football, Music, Fitness