

SHRAVAN GODSE

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EDUCATION

Carnegie Mellon University

Graduate Student, Mechanical Engineering

August '22 - Present

Pittsburgh, U.S.A.

- GPA: **4.0/4.0**

- Relevant Coursework: Molecular Simulations, Advanced Thermodynamics, Bayesian Machine Learning

Indian Institute of Technology, Bombay

Bachelor of Technology (with honors) in Mechanical Engineering

July '18 - May '22

Mumbai, India

- CPI: **9.02/10.00**

- Relevant Coursework: Thermodynamics, Heat Transfer, Lattice Dynamics, Intro. to Ab-initio Methods, Materials Informatics, Statistical Machine Learning and Data Mining, Deep Learning

- Minor in Management from Shailesh J. Mehta School of Management

PUBLICATIONS

G. Reuveni, Y. Diskin-Posner, C. Gehrman, **S. Godse**, et. al. "Static and Dynamic Disorder in Formamidinium Lead Bromide Single Crystals", [The Journal of Physical Chemistry Letters](#), 14, 5, 1288-1293 (2023)

S. Godse, Y. Srivastava and A. Jain, "Anharmonic lattice dynamics and thermal transport in type-I inorganic clathrates", [Journal of Physics: Condensed Matter](#), 34 145701 (2022)

A. Jain, H. P. Veeravankata, **S. Godse**, Y. Srivastava "High-throughput computational discovery of 40 ultralow thermal conductivity and 20 highly anisotropic crystalline materials", [ArXiv Preprint](#) (2022)

RESEARCH EXPERIENCE

EEG Lab

August '22 - Present

Guide: Prof. Venkat Viswanathan, Department of Mechanical Engineering

CMU, U.S.A.

As a graduate student researcher, working on Li-rich transition-metal oxide cathodes for Li-ion batteries using density functional theory (DFT) accelerated by scientific machine learning

- Reviewed literature on anionic redox for improving specific capacity/energy of Li-ion batteries
- Performed benchmark studies on Hubbard-U correction in DFT calculations on Li-transition metal oxides
- Currently working on training equivariant graph-neural-network potentials for Li-Ni-Mn-O system

Materials Research Lab

July '20 - May '22

Guide: Prof. Ankit Jain, Department of Mechanical Engineering

IIT Bombay, India

As an undergrad researcher, worked on multiple projects in DFT, lattice dynamics, nanoscale heat transfer and data-driven methods in materials science

1. Anharmonic lattice dynamics and thermal transport in type-I clathrates (Bachelor Thesis)

- Studied type-I clathrates $X_8Ga_{16}Ge_{30}$ (X: Sr/Ba) with potential applications in thermoelectricity
- Computed lattice thermal conductivities of , using inhouse ab-initio based anharmonic lattice dynamics code
- Employed techniques like renormalization, temperature dependent potential energy surface sampling and multichannel thermal transport to account for strong anharmonicity and wavelike phonon coherence

2. Machine learning for material property prediction

- Employed Symmetry Functions and Voronoi Tessellations to encode crystal structure and composition
- Implemented Farthest Point Sampling technique in Python for selecting most descriptive features
- Trained a neural network to predict formation energies of Al-Si-Mg alloys with a MAE of 0.02 eV/atom

Vibrational Spectra of FAPbBr₃

May '21 - August'21

Guide: Prof. David Egger, Department of Physics

TU Munich, Germany

- Investigated potential energy surface of FA⁺ in PbBr₃ environment and optimized hybrid perovskite structure
- Obtained phonon dispersion curves of FAPbBr₃ using PhonoPy with finite difference method
- Simulated infrared and Raman spectra of FAPbBr₃ using VASP and PhonoPy-Spectroscopy modules

TECHNICAL SKILLS

Languages : Python, MATLAB, C++, HTML*, CSS* (*basic proficiency)

Softwares and Packages : Pytorch, Keras, Scikit-Learn, NumPy, Simulink

Materials Simulation/Querying : Quantum Espresso, VASP, LAMMPS, PhonoPy, ASE, Pymatgen

Others : Autocad, \LaTeX , Fusion 360, Inkscape, Photoshop

INDUSTRY EXPERIENCE

Research Intern | QPiVolta Technologies

January - April '22

QPivolta is an emerging start-up working at the intersection of AI and solid-state batteries

- Trained a graph neural network model, GemNet, on molecular simulation data for a solid Li-ion conductor
- Developed a Python interface for accelerating ab-initio molecular simulations harnessing graph neural network models on the Open Catalyst Project

Advance Engineering Intern | Varroc Engineering Ltd.

December '19

Varroc is a global technology powerhouse in manufacturing and supplying automotive components

- Researched various charging strategies for **Lithium-ion batteries** for Electric Vehicle applications
- Studied and presented Constant Current-Constant Voltage (CC-CV), Multistage, Pulsed and Fuzzy Control based charging of lithium-ion batteries based on literature reviews
- Modeled CC-CV and Multistage charging in **Simulink** to compare for an optimal charging profile

KEY COURSE PROJECTS

Non-uniform meshed Schrodinger-Poisson

Autumn '20

Instructor: Prof. Dipankar Saha, Department of Electrical Engineering

IIT Bombay

- Obtained a 99.64% accuracy with $1/10^{\text{th}}$ computational resources upon solving Schrodinger equation using the technique of non-uniform mesh by [Tan et al.](#) for a finite quantum well using Python
- Implemented the self-consistent Schrodinger-Poisson equation to obtain carrier densities in AlGaAs and GaAs

BiDet-binarized object detector

Autumn '20

Instructor: Prof. P. Balamurugan, Department of IEOR

IIT Bombay

- Worked in a team of 4 and used a binarized neural network Bidet by [Wang et al.](#) for object detection
- Experimented on PASCAL-VOC and COCO datasets for training and testing the object detector

GCMC simulations of $\text{Li}_3\text{V}_2\text{O}_5$

Fall '22

Instructor: Prof. Gerald Wang, Department of Civil & Environmental Engineering

CMU

- Employed state-of-the-art Neural Equivariant potential (Nequip) and investigated the disordered rock-salt - $\text{Li}_3\text{V}_2\text{O}_5$ as a potential anode material for Li-ion batteries
- Ran grand canonical monte-carlo simulations to obtain open-circuit voltage profile

SCHOLASTIC ACHIEVEMENTS

- Awarded **Undergraduate Research Award** for contributions to research in lattice dynamics ['21]
- Secured **All India Rank 1242** among **2 lakh** candidates in **JEE Advanced** for admission to IITs ['18]
- Secured **All India Rank 3433** among **1.1 million** in **JEE Main** entrance exam ['18]
- Selected for **Indian National Olympiads** in **Physics** and **Astronomy** by being in **top 1%** in India ['18]
- Recipient of the prestigious **Kishore Vaigyanik Protsahan Yojana (KVPY) scholarship**, a national fellowship awarded by Dept. of Science & Technology, Government of India for students with an aptitude in research ['18]
- Recipient of the Scholarship for Higher Education (SHE), a part of **Inspire scheme** by Dept. of Science & Technology for performance in **top 1%** in class XII board examinations ['18]

MENTORSHIP ROLES

Institute Student Mentor

June '21 - May '22

Institute Student Mentorship Program

IIT Bombay

- Part of a 133-member team selected out of 300+ applicants on the basis of **overall performance** in the institute via a rigorous procedure of SoPs, interviews and peer reviews
- Responsible for mentoring **12 freshmen**, aiding them adjust to academics and life at IIT Bombay

Department Academic Mentor

July '20 - May '21

Department Academic Mentorship Program

IIT Bombay

- Mentored **6** sophomores in the department to provide **academic guidance** and general counsel
- Conducted a **help-session** on basic solid state physics for sophomores to get clarity in concepts

EXTRACURRICULAR ACTIVITIES

- Volunteered at **Krittika**, the **Astronomy Club** of IIT Bombay, conducting star gazing activities and lectures
- Finished year long training in **Swimming** under National Sports Organization (NSO)
- Completed 3 levels of **Indian Classical Music** (Vocals) and 1 level of Harmonium (Indian Classical)
- Completed Fit in Deutsch 1 (A1 level proficiency in **German** language) conducted by Goethe Institut