

SHRAVAN GODSE

☎ (+91) 7888049790 ✉ Email 🔗 LinkedIn 📄 Google Scholar 🏠 Homepage

EDUCATION

Indian Institute of Technology, Bombay

July '18 - May '22 (expected)

Bachelor of Technology (with honors) in Mechanical Engineering

Mumbai, India

- CPI (after 7 semesters) : **9.0/10**

- Pursuing a minor in Management from Shailesh J. Mehta School of Management

PUBLICATION

Shravan Godse, Yagyank Srivastava and Ankit Jain, "Anharmonic lattice dynamics and thermal transport in type-I inorganic clathrates", *Journal of Physics: Condensed Matter* **34(14)**, 145701 (2022)

RESEARCH EXPERIENCE

Materials Research Lab

July '20 - Present

Guide: Prof. Ankit Jain, Department of Mechanical Engineering

IIT Bombay

As an undergrad researcher, working on multiple projects in density functional theory (DFT), lattice dynamics, nanoscale thermal transport and data-driven methods in materials science

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

- Computed lattice thermal conductivities of type-I clathrates $X_8\text{Ga}_{16}\text{Ge}_{30}$ (X: Sr/Ba), using inhouse **ab-initio** based anharmonic lattice dynamics code on spacetime **supercomputing** facility at IIT Bombay
- Employed techniques like **renormalization**, temperature dependent potential energy surface sampling and **multichannel thermal transport** to account for strong anharmonicity and wavelike phonon coherence
- Obtained temperature-dependent phonon dispersion curves, density of states, atomic displacement parameters
- Obtained **DFT potential energy surface** and force-field around Ba/Sr atoms in tetrakaidecahedral cages

2. Machine learning for material property prediction (Bachelor Thesis-II, ongoing)

- 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**
- Currently working on predicting lattice dynamical properties using **random forests** and neural networks

Vibrational Spectra of FAPbBr₃

May '21 - August '21

Guide: Prof. David Egger, Department of Physics

TU Munich

Worked on the hybrid perovskite **FAPbBr₃** and obtained its lattice dynamical properties using DFT

- Investigated potential energy surface of FA^+ in PbBr_3 environment and optimized hybrid perovskite structure
- Reviewed and performed Van-der Waals corrections using **Tkatchenko-Scheffler** method in **VASP**
- Obtained phonon dispersion curves of Si, GaAs and FAPbBr₃ using **PhonoPy** with finite difference method
- Simulated **infrared and Raman spectra** of FAPbBr₃ using VASP and PhonoPy-Spectroscopy modules

Materials Simulation

April '20 - July '20

Guide: Prof. Dipanshu Bansal, Department of Mechanical Engineering

IIT Bombay

Simulated **Bandstructure**, Density of states and **Phonon Dispersions** of materials using DFT software

- Reviewed concepts in solid state physics and completed an online course on Density Functional Theory
- Performed SCF calculations for convergences with respect to energy cutoffs and k point sampling
- Obtained bandstructure and phonon dispersion curves for **Al** and **Si** using **Quantum Espresso**
- Obtained the density of states (total and orbital projected) using dos.x and projwfc.x modules in Espresso

INDUSTRY EXPERIENCE

Advance Engineering Intern | Varroc Engineering Ltd.

December '19

Guide: Mr. Lohit Dhamija - Manager, Advanced Engineering

Pune

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

TECHNICAL SKILLS

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

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

Materials Simulation/Querying : Quantum Espresso, VASP, Phonopy ASE, Matminer, Pymatgen

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

KEY COURSE PROJECTS

Non-uniform meshed Schrodinger-Poisson | Report

Autumn '20

Instructor: Prof. Dipankar Saha, Department of Electrical Engineering

IIT Bombay

- Obtained a **99.64% accuracy** with **1/10th 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 | Report

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

Benzene Molecule Simulation | Report

Autumn '20

Instructor: Prof. Sumit Saxena, Department of Materials Science

IIT Bombay

- Utilised **Quantum Espresso** to carry out Density Functional Theory calculations on **Benzene molecule**
- Performed self consistent calculations using pw.x module and visualized the **molecular orbitals** of Benzene

SCHOLASTIC ACHIEVEMENTS

- Awarded **Undergraduate Research Award** for contributions to research in lattice dynamics ['21]
- Awarded a **branch change** based on exemplary academic performance in freshman year at IIT Bombay ['19]
- 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]

KEY COURSES

Mechanical Engineering Curriculum*	Fluid Mechanics, Solid Mechanics, Thermodynamics, Heat Transfer Mechanical Measurements, Manufacturing Processes
Machine Learning, Math	Deep Learning - Theory and Practice, Statistical Machine Learning and Data Mining, Linear Algebra, Multivariable Calculus
Physics, Materials Science	Quantum Physics, Physics of Nanoelectronic Devices, Introduction to Ab-initio Methods, Lattice Dynamics and Thermal Transport

*accompanied by lab courses

MENTORSHIP ROLES

Institute Student Mentor

June '21 - Present

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**) conducted by Goethe Institut

REFERENCES

Prof. Ankit Jain Materials Research Lab Department of Mechanical Engg. IIT Bombay a_jain@iitb.ac.in	Prof. David Egger TheoFEM Lab Department of Physics TU Munich, Germany david.egger@tum.de	Prof. Dipanshu Bansal Vibrational Spectroscopy Lab Department of Mechanical Engg. IIT Bombay dipanshu@iitb.ac.in
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