

# SHRAVAN GODSE

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## EDUCATION

### Indian Institute of Technology, Bombay

Bachelor of Technology (with honors) in Mechanical Engineering

- CPI (after 6 semesters) : **8.97/10**

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

July '18 - May '22 (expected)  
Mumbai, India

## PUBLICATION

**S. Godse**, Y. Srivastava, A. Jain; *Anharmonic lattice dynamics and thermal transport in type-I inorganic clathrates* (submitted to J. Phys. Condens. Matter) [[Preprint- arXiv:2110.13183](#)]

## 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) based lattice dynamics, nanoscale thermal transport and material fingerprinting for machine learning enabled materials discovery

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

- Computed lattice thermal conductivities of type-I clathrates  $X_8Ga_{16}Ge_{30}$  (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 FAPbBr<sub>3</sub>

May '21 - August '21

Guide: Prof. David Egger | Department of Physics

TU Munich

Worked on the hybrid perovskite **FAPbBr<sub>3</sub>** 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 FAPbBr<sub>3</sub> using **PhonoPy** with finite difference method
- Simulated **infrared and Raman spectra** of FAPbBr<sub>3</sub> 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
- Modelled 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

**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 **1/10<sup>th</sup> 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 a merit-based **branch change** based on exemplary academic performance in the first year [ '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]
- Awarded **Undergraduate Research Award** for contributions to research in lattice dynamics [ '21]
- Qualified 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

<b>Mechanical Engineering Curriculum*</b>	Fluid Mechanics, Solid Mechanics, Thermodynamics, Heat Transfer Mechanical Measurements, Manufacturing Processes
<b>Machine Learning, Math</b>	Deep Learning-Theory and Practice, Statistical Machine Learning and Data Mining, Linear Algebra, Multivariable Calculus
<b>Physics, Materials Science</b>	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 a group of incoming freshmen aiding them adjust to 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

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