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

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), 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 $X_8Ga_{16}Ge_{30}$ (X: Sr/Ba), using inhouse **ab-inito** 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 $FAPbBr_3$ *May '21 - August'21*
Guide: Prof. David Egger, Department of Physics *TU Munich*
Worked on the hybrid perovskite **$FAPbBr_3$** 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 $FAPbBr_3$ using **PhonoPy** with finite difference method
- Simulated **infrared and Raman spectra** of $FAPbBr_3$ 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 Eduaction (**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-inito 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	**Prof. David Egger**	**Prof. Dipanshu Bansal**
Materials Research Lab	TheoFEM Lab	Vibrational Spectroscopy Lab
Department of Mechanical Engg.	Department of Physics	Department of Mechanical Engg.
IIT Bombay	TU Munich, Germany	IIT Bombay
a_jain@iitb.ac.in	david.egger@tum.de	dipanshu@iitb.ac.in