Shravan Godse

(+91) 7888049790 shravan.godse@iitb.ac.in LinkedIn Homepage

Materials for Energy, Computational Materials Science, Nanoscale Thermal Transport

Education

Indian Institute of Technology, Bombay *July '18 - May '22 (expected)*
Bachelor of Technology (with honors) in Mechanical Engineering *Mumbai, India*
- CPI (after 6 semesters) : **8.97/10**
- Pursuing a minor in Management from Shailesh J. Mehta School of Management

Publication

Godse S., Srivastava Y., Jain A.
Anharmonic lattice dynamics and thermal transport in type-I inorganic clathrates (2021) [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-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
- 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 **1/10th 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 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]
- Amongst **top 1 %** students in **National Standard Examination in Physics** and **National Standard Examination in Astronomy** conducted by Indian Association of Physics Teachers ['18]
- Recipient of the prestigious **Kishore Vaigyanik Protsahan Yojana (KVPY) scholarship**, a national fellowship awarded by Dept. of Science & Technology, Government of India ['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 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

- Volunteering at National Service Scheme's, **Open Learning Initiative**, creating free educational content in local languages for underprivileged school students in the state of Maharashtra
- 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