Shravan Godse

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Education

Carnegie Mellon University *August '22 - Present*
Graduate Student, Mechanical Engineering *Pittsburgh, U.S.A.*
- GPA: **4.0/4.0**
- Relevant Coursework: Bayesian Machine Learning, Molecular Simulations, Advanced Thermodynamics

Indian Institute of Technology, Bombay *July '18 - May '22*
Bachelor of Technology (with honors) in Mechanical Engineering *Mumbai, India*
- CPI: **9.02/10.00**
- Relevant Coursework: Thermodynamics, Fluid Mechanics, Machine Design, Heat Transfer, Lattice Dynamics, 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. Gehrmann, **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. Veeravenkata, **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*
PI: 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

- Performed an extensive literature review on anionic redox for improving specific capacity of Li-ion batteries
- Currently developing high-fidelity **equivariant graph neural network** potentials for Li-Ni-Mn-O system

Materials Research Lab *July '20 - May '22*
PI: Prof. Ankit Jain, Department of Mechanical Engineering *IIT Bombay, India*

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 from first-principles methods on SpaceTime **supercomputing** facility
   - Employed techniques like **phonon renormalization** and **multichannel thermal transport** to account for higher order effects and diffusive heat transfer at nanoscale
2. *Machine learning for material property prediction*
   - Employed **feature engineering** methods such as Symmetry Functions and Voronoi tessallations for crystals
   - 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**

TheoFEM Lab *May '21 - August'21*
PI: Prof. David Egger, Department of Physics *TU Munich, Germany*
- Worked on hybrid organic-inorganic perovskite $FAPbBr_3$ with applications **solar cells**
- Elucidated disorder of FA^+ by mapping potential energy surface using **VASP**
- Simulated infrared and **Raman spectra** of $FAPbBr_3$ 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	: Docker, Autocad, LaTeX, Fusion 360, Inkscape, Photoshop

Industry Experience

Research Intern | **QPiVolta Technologies Pvt. Ltd.** *January - April '22*

QPiVolta is a leading start-up working at the intersection of AI and solid-state batteries

- Compiled and containerized **GPU**-version of Quantum Espresso on **Amazon Web Services** using **Docker**
- Trained a graph neural network model, **GemNet**, on molecular simulation data for a solid Li-ion conductor
- Developed a Python interface for accelerating ab-inito molecular simulations through **active learning** using 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

Academic Projects

Data-driven Inverse Airfoil Design *Fall '22*
Bayesian Machine Learning *CMU*

- Designed a **convolutional** neural net in **PyTorch** to predict lift-drag coefficients with an R^2 score of **0.98**
- Trained a **generative adversarial neural network** and created a pipeline for **inverse design** of airfoils

Optimizing Formula1 Racing Line *Fall '22*
Numerical Methods *CMU*

- Employed the **differentiable** PyTorch framework to optimize F1 raceline using **gradient descent** algorithm
- Compared stability of different gradient descent variants such as **momentum** and **adaptive momentum (ADAM)**

GCMC simulations of $Li_3V_2O_5$ *Fall '22*
Molecular Simulations *CMU*

- Employed state-of-the-art Neural Equivariant interatomic potential (NequIP) and investigated the disordered rock-salt - $Li_3V_2O_5$ as a potential anode material for Li-ion batteries
- Ran **grand canonical monte-carlo** simulations to obtain convex hull and open-circuit voltages

Non-uniform meshed Schrodinger-Poisson Solver *Autumn '20*
Physics of Nanoelectronic Devices *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 *Autumn '20*
Deep Learning *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

Scholastic Achievements

- Awarded **Narotam Sekhsaria Scholarship** (INR 1 lakh) for excellent aptitude in academics and research [*'21*]
- Awarded **Undergraduate Research Award** for contributions to research in lattice dynamics [*'21*]
- 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*]

Extracurricular Activities

- Actively involved in mentoring students at IIT Bombay as a part of the **Institute Student Mentorship Program**
- 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, Pune