SRIHARI MADHAV KASTUAR

Department of Physics, Lehigh University
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Career Objective

My research focuses on the computational design and discovery of next-generation solid state materials, aiming for innovative and sustainable technological applications. I study the fundamental physics of low-dimensional materials, renowned for their emergent quantum phenomena, while harnessing advanced data-driven machine learning techniques to characterize new materials with tailored properties on a large scale. Through my research I hope to contribute to the scientific understanding and development of energy-efficient solutions for a sustainable future.

EXPERIENCE (RESEARCH AND TEACHING):

Teaching Assistant/Grader **2024 - present**

Department of Physics, Lehigh University, Bethlehem, PA.

- Course: Introduction to Modern Physics (PHY – 031)

Research Fellow **2022 - present**

Dr. Hyo Sang Lee Graduate Fellow, Department of Physics, Lehigh University, Bethlehem, PA.

- Engineered intermediate band states in two-dimensional (2D) heterostructures of group IV monochalcogenides via copper intercalation for next-generation solar cell devices with quantum efficiencies as high as 190 %.
- Developed a computational framework to design novel intercalated 2D/organic hybrid materials using high-throughput density functional theory computations along with materials modeling and active learning. *In collaboration with Dr. Srinivas Rangarajan, Department of Chemical and Biomolecular Engineering, Lehigh University.*

Research Assistant **2021 - 2022**

Department of Physics, Lehigh University, Bethlehem, PA.

- First principles investigation of next-generation lead-free perovskite derived family of 2D materials, and the strain-engineered tunabilty of their optoelectronic structure.

Research Fellow **2020 - 2021**

Dr. Hyo Sang Lee Graduate Fellow, Department of Physics, Lehigh University, Bethlehem, PA.

- Developed a machine learning model to predict structure-property relations of over 10,000 2D materials characterized on the basis of their elastic and lattice constants.
- First-principles study of the electronic properties of 2D MoS_2 using classical molecular dynamics simulations.
- First-principles study of the electronic properties of ZnO and CuO using density functional theory.

Subject Matter Expert and Quality Analyst **2019 - 2020**

Evelyn Learning Private Limited, India.

- Led a team of ten in developing advanced physics related content for various schools and online publishers, both Indian and foreign, and was recognized for “solving most complex problems” via a *Aryabhatta Award* in two consecutive quarters.

Graduate Student **2017 - 2019**

National Institute of Technology, Calicut, India.

- First-principles study of lithium-decorated black phosphorene for efficient hydrogen storage.

Physics Tutor **2014 - 2016**

New Delhi, India.

- Taught 9th and 10th standard physics to four high school students.

EDUCATION:

M.Sc. Physics **August 2019**

National Institute of Technology, Calicut, India.

- **Thesis**: Ab-initio studies of hydrogen adsorption on lithium decorated defective black phosphorene using density functional theory.
- **Advisor**: Dr. Raghu Chatanathodi

B.Sc. Physics **July 2016**

University of Delhi, New Delhi, India.

SKILLS/SOFTWARE/PERSONALS:

Scientific software:	VASP, Quantum Espresso, LAMMPS, Wannier90, WannierTools, LaTeX.
Operating systems:	Linux, Mac, Windows.
Languages:	Python, Mathematica, MATLAB, Bash shell scripting.
Personals:	Scientific writing, presentation, and editing; Indian classical dance; music editing and composition; song writing; and playing acoustic/electric guitar.

PUBLICATIONS:

Citations: ~ 32, source: Google Scholar

- **Kastuar, S. M.**, Rzepa, C., Rangarajan, S. Ekuma, C. E. (2024). A high-throughput and data-driven computational framework for novel quantum materials. *Digital Discovery (under peer review).*
- **Kastuar, S. M.**, Ekuma, C. E. (2024). Chemically Tuned Intermediate Band States in Atomically Thin Cu_xGeSe/SnS Quantum Material for Photovoltaic Applications. *Science Advances (accepted).*
- Khanmohammadi S., Kushnir, K., Chen, E., **Kastuar, S. M.**, Ekuma, C. E., Koski, K. J., Titova, L. V. (2024). Tailoring Ultrafast Near Band Gap Photoconductive Response in GeS by Zero-Valent Cu Intercalation. *Applied Materials and Interfaces (accepted).*
- **Kastuar, S. M.**, Liu, Z. L., Najmaei, S., Ekuma, C. E. (2023). Mechanical properties of cubic boron nitride and diamond at dynamical pressure and temperature. *Applied Physics Letters*, *123*(23).
- Lalrinkima, **Kastuar, S. M.**, Zadeng, L., Zosiamliana, R., Chettri, B., Singh, Y. T., Zuala, L., Rai, D. P., Ekuma, C. E. (2023). Giant intrinsic magnetoresistance in spin-filtered tunnel junctions with ferrimagnetic electrode. *Physical Review B*, *107*(15), 155305.
- **Kastuar, S. M.**, Ekuma, C. E. (2023). Giant electrophotonic response in two-dimensional halide perovskite Cs 3 Bi 2 I 9 by strain engineering. *Physical Review Materials*, *7*(2), 024002.
- **Kastuar, S. M.**, Ekuma, C. E., Liu, Z. L. (2022). Efficient prediction of temperature-dependent elastic and mechanical properties of 2D materials. *Scientific Reports*, *12*(1), 3776.
- John, D., Nharangatt, B., **Kastuar, S. M.**, Chatanathodi, R. (2021). Blue phosphorene nanosheets with point defects: Electronic structure and hydrogen storage capability. *Applied Surface Science*, *551*, 149363.

CONFERENCE PRESENTATIONS:

1. **Srihari Kastuar**, Chinedu Ekuma, and Sina Najmaei. "Computational Synthesis of Perovskene Quantum Materials." APS March Meeting 2024, March 08, Minneapolis.

2. **Srihari Kastuar** and Chinedu Ekuma. "Large excitonic effects in 2D $Cs_3Bi_2I_{9-x}Cl_x$ perovskites." APS March Meeting 2024, March 06, Minneapolis.
3. **Srihari Kastuar**, Lyubov Titova, Kristie Koski, and Chinedu Ekuma. "Many-body effects-driven intermediate band states in intercalated 2D Cu_xGeSe/SnS heterostructure." APS Mid-Atlantic Section 2023, November 04, University of Delaware.
4. **Srihari Kastuar**, Christopher Rzepa, Chinedu Ekuma, and Srinivas Rangarajan. "A computational framework accompanied by machine learning techniques for designing two-dimensional/organic hybrid quantum materials." APS March Meeting 2023, March 08, Las Vegas.
5. **Srihari Kastuar**, and Chinedu Ekuma. "Engineering intermediate band states in Cu-intercalated 2D transition metal chalcogenides." APS March Meeting 2023, March 06, Las Vegas.
6. **Srihari Kastuar**, Chinedu Ekuma, Christopher Rzepa, Srinivas Rangarajan, and Zhong-Li Liu. "Machine Learning-guided Design of Emerging 2D-based Materials." APS Mid-Atlantic Section 2022, December 04, Pennsylvania State University (**Invited speaker**).
7. **Srihari Kastuar**, Chinedu Ekuma, and Zhong-Li Liu. "Ab initio modeling of lead-free perovskite-derived 2D $Cs_3Bi_2I_9$." APS March Meeting 2022, March 15, Chicago.