SRIHARI M. KASTUAR

smk520@lehigh.edu +1 (484) 767-1658

Department of Physics, Lehigh University
16 Memorial Drive East
Bethlehem, PA 18015

RESEARCH SUMMARY

I am a computational condensed matter physicist. My research focuses on the computational design and discovery of *quantum materials* for applications in next-generation sustainable technology and devices. I study the fundamental physics of two-dimensional materials, and their heterostructures, 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 aim to contribute to the scientific understanding and development of energy-efficient solutions for a sustainable future.

EXPERIENCE (RESEARCH AND TEACHING):

Research/Teaching Assistant **2024 - present**

Department of Physics, Lehigh University, Bethlehem, PA.

- Course: Introduction to Modern Physics (PHY 031)
- Course: Methods of Mathematical Physics (PHY 428)

Research Fellow **2022 - 2024**

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 %. ***Listen to Gemini LLM-generated Podcast on this work.***
- Developed a computational framework to design novel intercalated 2D/organic hybrid materials using high-throughput density functional theory and reinforcement learning. Co PI - 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 graduate level physicists in developing graduate level physics content, which also wrote the complete solutions to "*Introduction to Electrodynamics*" *by David J. Griffiths*. Solved various numerical questions related to physics and interdisciplinary subjects like astrophysics and mechanical

engineering, and was recognized for *"solving most complex problems"* via an *Aryabhata 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:	VASP, Quantum Espresso, Wannier90, WannierTools, LAMMPS, xmgrace, LaTeX
Operating systems:	Linux, Mac, Windows
Languages:	Python, bash
Personals:	Scientific writing, presentation, and editing; Indian classical dance; music writing, editing and composition; and playing acoustic/electric guitar.

PUBLICATIONS:

Source: Google Scholar

- Iloanya, A. C., **Kastuar**, **S. M.** and Ekuma, C. E. Tailoring electrophotonic capabilities of atomically thin GeS through controlled organometallic intercalation. *Journal of Applied Physics* 136.8 (2024).
- **Kastuar, S. M.**, Rzepa, C., Rangarajan, S. Ekuma, C. E. A high-throughput and data-driven computational framework for novel quantum materials. *arXiv preprint arXiv:2406.15630* (2024).
- **Kastuar, S. M.**, Ekuma, C. E. Chemically Tuned Intermediate Band States in Atomically Thin Cu_xGeSe/SnS Quantum Material for Photovoltaic Applications. *Science Advances*, *10*(15), eadl6752 (2024). ***Listen to AI generated podcast.***
- Khanmohammadi S., Kushnir, K., Chen, E., **Kastuar, S. M.**, Ekuma, C. E., Koski, K. J., Titova, L. V. Tailoring Ultrafast Near Band Gap Photoconductive Response in GeS by Zero-Valent Cu Intercalation. *ACS Applied Materials and Interfaces* (2024).
- **Kastuar, S. M.**, Liu, Z. L., Najmaei, S., Ekuma, C. E. Mechanical properties of cubic boron nitride and diamond at dynamical pressure and temperature. *Applied Physics Letters*, *123*(23) (2023).
- Lalrinkima, **Kastuar, S. M.**, Zadeng, L., Zosiamliana, R., Chettri, B., Singh, Y. T., Zuala, L., Rai, D. P., Ekuma, C. E. Giant intrinsic magnetoresistance in spin-filtered tunnel junctions with ferrimagnetic electrode. *Physical Review B*, *107*(15), 155305 (2023).
- **Kastuar, S. M.**, Ekuma, C. E. Giant electrophotonic response in two-dimensional halide perovskite Cs 3 Bi 2 I 9 by strain engineering. *Physical Review Materials*, *7*(2), 024002 (2023).
- **Kastuar, S. M.**, Ekuma, C. E., Liu, Z. L. Efficient prediction of temperature-dependent elastic and mechanical properties of 2D materials. *Scientific Reports*, *12*(1), 3776 (2022).
- John, D., Nharangatt, B., **Kastuar, S. M.**, Chatanathodi, R. Blue phosphorene nanosheets with point defects: Electronic structure and hydrogen storage capability. *Applied Surface Science*, *551*, 149363 (2021).

INVITED TALK:

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.

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, and Zhong-Li Liu. "Ab initio modeling of lead-free perovskite-derived 2D $Cs_3Bi_2I_9$." APS March Meeting 2022, March 15, Chicago.