SRIHARI M. KASTUAR

kastus@rpi.edu +1 (484) 767-1658
sm.kastuar@gmail.com

Center for Biotechnology and Interdisciplinary Studies
Rensselaer Polytechnic Institute, Troy, New York, 12180

Computational materials physicist developing first-principles, high-throughput, and data-driven approaches for discovering and understanding 2D quantum materials. Expertise in electronic-structure theory, alloy thermodynamics, machine learning, and high-performance computing.

Keywords: Computational quantum materials; 2D materials; first-principles electronic structure; high-throughput materials discovery; Monte Carlo simulations; thermodynamic integration; machine learning and inverse design; topological and magnetic materials; tight-binding

EDUCATION:

Ph.D. Physics August 2025
Lehigh University, Bethlehem, Pennsylvania, USA.
- Thesis: *Data-driven design of two-dimensional quantum materials*.
- Advisor: Chinedu Ekuma

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: Raghu Chatanathodi

AWARDS:

Dr. Hyo Sang Lee Graduate Fellowship Highly competitive multi-year fellowship awarded to up to 3 graduate students per year (full tuition, stipend ~ $36,000 p.a.)
Lehigh University, Bethlehem, PA, USA

GERA Travel Grant $500 to attend 2025 APS March Meeting
American Physical Society

EXPERIENCE (RESEARCH AND TEACHING):

Postdoctoral Research Associate March 2026 to present
Rensselaer Polytechnic Institute, Troy, New York.
- Developed cluster-expansion models for 2D $Mo(S,Te)_2$ and 3D (Al,Ga)N and (Al,Sc)N alloys. Built a computational framework integrating high-throughput DFT, active learning, uncertainty quantification, and Monte Carlo sampling for efficient exploration of large configurational spaces, and applied statistical thermodynamics and thermodynamic integration to predict finite-temperature phase stability and construct binodal and spinodal phase boundaries.

Postdoctoral Researcher August 2025 to February 2026
Department of Physics, Boston College, Chestnut Hill, MA.
- Developed and implemented tight-binding models for 2D moiré quantum materials, including monolayer, bilayer, and trilayer graphene; twisted bilayer graphene; graphene/hBN; and multilayer graphene/hBN heterostructures with lattice mismatch and twist. Extracted tight-binding Hamiltonian parameters from first-principles calculations using Wannier90 and reproduced electronic structures reported in the literature.

Developed a computational workflow to construct periodic commensurate supercells of twisted 2D heterostructures for direct DFT calculations.

Research/Teaching Assistant 2024 - 2025

Department of Physics, Lehigh University, Bethlehem, PA.

- High-throughput discovery of stable 2D topological Heusler alloys (Heuslerenes). Computationally exfoliated ~800 monolayers from bulk full- and half-Heusler compounds and screened them for energetic and mechanical stability. Characterized topological and magnetic phases using first-principles calculations and Wannier charge-center analysis. Investigated candidate excitonic-insulator phases using GW-BSE. Mentored an undergraduate researcher in developing a representation-learning workflow to cluster materials based on their electronic band structures.
- Impurity induced magnetism in two-dimensional germanium sulfide – adsorption of atomic hydrogen.
- Course graded: Introduction to Modern Physics (PHY 031)
- Course graded: Methods of Mathematical Physics (PHY 428)
- Mentored three undergraduate students, Justin Hart, Tianhao Lian and Athiel Mading, in electronic structure calculations and machine learning. Athiel won the *best poster* award in an annual materials symposium organised by the Institute of Functional Materials and Devices at Lehigh University (2024). Tianhao has authored papers published in ACS Omega (2024) and Journal of Applied Physics (2025). Justin has authored a paper published in APL Materials (2025).

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%.
- Developed a computational framework to design novel intercalated 2D/organic hybrid materials using high-throughput density functional theory and reinforcement learning.

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 tunability 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 based on their elastic and lattice constants.
- Molecular dynamics study of 2D MoS_2 using the REBO potential.
- First-principles study of the electronic properties of ZnO and CuO using density functional theory with Hubbard U correction.

Subject Matter Expert and Quality Analyst 2019 - 2020

Evelyn Learning Private Limited, India.

- Led a team of ten physicists in developing graduate level physics content, and curated *complete* solutions to "*Introduction to Electrodynamics*" *by David J. Griffiths*. Solved various numerical/computational 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.

COMPUTATIONAL SKILLS:

Electronic Structure:	VASP, Quantum ESPRESSO, Wannier90, WannierTools; DFT, DFT+U, hybrid DFT, GW-BSE, spin-orbit coupling, tight-binding.
Materials Modeling:	Cluster expansion, Monte Carlo, thermodynamic integration, AIMD
ML/Data:	scikit-learn, PyTorch, active learning, reinforcement learning, uncertainty quantification, materials informatics.
Programming/HPC:	Python, Git, Bash, Linux, SLURM; automated high-throughput workflows and large-scale parallel first-principles calculations.

INVITED TALK:

"Machine Learning-guided Design of Emerging 2D-based Materials." Srihari Kastuar, Chinedu Ekuma, Christopher Rzepa, Srinivas Rangarajan, and Zhong-Li Liu. *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.

PUBLICATIONS:

Source: Google Scholar

- **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).
- **Kastuar, S. M.**, & Ekuma, C. E. Large exciton binding energy in atomically thin Cs3Bi2I9-xClx halide perovskite. *Computational Materials Science*, *253*, 113827 (2025).
- Hart, J. B., **Kastuar, S. M.**, Iloanya, A. C., & Ekuma, C. E. High-throughput discovery of topological and magnetic phases in Heuslerenes. *APL Materials*, *13*(11) (2025).
- Cid, B. J., **Kastuar, S. M.**, Iloanya, A. C., Rangarajan, S., & Ekuma, C. E. Ab initio elucidation of PTCDA intercalation mechanism in MoS2 bilayer. *npj 2D Materials and Applications*, *9*(1), 80 (2025).
- Lian, T., Iloanya, A. C., **Kastuar, S. M.**, Jana, G., & Ekuma, C. E. Defect-induced bipolar magnetism in atomically thin GeS. *Journal of Applied Physics*, *137*(23) (2025).
- **Kastuar, S. M.**, Rzepa, C., Rangarajan, S., & Ekuma, C. E. A high-throughput and data-driven computational framework for novel quantum materials. *APL Mach. Learn.* 2, 046108 (2024).

- **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).

- **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).

- Iloanya, A. C., **Kastuar, S.M.**, Jana, G., & Ekuma, C. E. Atomic-scale intercalation and defect engineering for enhanced magnetism and optoelectronic properties in atomically thin GeS. *Scientific Reports,* 15, 4546 (2025).

- Lian, T., Iloanya, A. C., **Kastuar, S. M.**, Tayo, B. O., & Ekuma, C. E. p-Type Sensing of DNA Nucleobases Adsorbed on Graphene Nanoribbon. *ACS Omega*, (2024).

- 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).

- Iloanya, A. C., **Kastuar**, **S. M., &** Ekuma, C. E. Tailoring electrophotonic capabilities of atomically thin GeS through controlled organometallic intercalation. *Journal of Applied Physics* 136.8 (2024).

- 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).

- 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).

REFEREES:

Available upon request