Akram Ibrahim, M.S.

Baltimore, MD 21227
Mobile: +1 443 851 3047
Email: akrami1@umbc.edu

EDUCATION

University of Maryland Baltimore County February 2025 (**Expected**)
Department of Physics
Baltimore, MD, USA
Doctor of Philosophy (Ph.D.) in Physics (computational materials science)

- Thesis: Understanding growth of low-dimensional materials using multiscale modeling and machine learning
- Supervisor: **Dr. Can Ataca**

University of Maryland Baltimore County May 2021
Department of Physics
Baltimore, MD, USA
Master of Science (M.S.) enroute to Ph.D. in Physics

- GPA: 3.9/4

Menoufia University July 2016
Department of Mechanical Power Engineering
Menoufia, Egypt
Bachelor of science (B.Sc.) in Mechanical Engineering

- GPA: 3.8/4 (Top 1%)
- Thesis: Experimental design and finite element simulation of a double-pipe heat exchanger with variable-geometry turbulence-induction mechanism

WORK EXPERIENCE

SAMSUNG SEMICONDUCTOR, INC. June 2024 – August 2024
Advanced Materials Lab
Cambridge, MA, USA
Intern, Computational Semiconductor Research

- **Project: Hybrid Kinetic Monte Carlo (KMC) and Molecular Dynamics (MD) Simulation for Amorphous Boron Nitride (aBN) Growth Using Machine Learning Potentials**
  Developed "KMCPACK," a Python package within the Atomic Simulation Environment (ASE) for hybrid KMC and MD simulations, facilitating custom event definition and processing for the growth of amorphous materials; implemented a neural network potential (NNP) for aBN growth and benchmarked results against TEM experiments, identifying structural motifs crucial for its ultra-low dielectric constant.
- Supervisor: **Dr. Yongwoo Shin**

University of Maryland Baltimore County June 2022 – present
Department of Physics
Baltimore, MD, USA
Research Assistant

- **Project (1): Comprehensive Study of Lithium Adsorption and Diffusion on Janus Mo/WXY (X, Y = S, Se, Te) Using First-Principles and Machine Learning Approaches**
  Designed physics-based descriptors for Li adsorption process and applied cluster-wise linear regression to predict Li adsorption energies on two-dimensional (2D) regular/Janus transition metal dichalcogenides at varying Li concentrations.

- **Project (2): Modeling Chemical Exfoliation of Non-Van der Waals (vdW) Chromium Sulfides by Machine Learning Interatomic Potentials and Monte Carlo Simulations**
  Developed a NNP for nonstoichiometric disordered environments in chemically exfoliated non-vdW materials; analyzed its generalization for configurational and geometric optimization against cluster expansion; utilized the NNP for simulated annealing to predict $Cr_{(1-x)}S$ crystal structures and in vacancy diffusion Monte Carlo (MC) to study non-vdW to vdW phase transition under lateral strain.

- **Project (3): Modeling Defect Dynamics in MoS_2 Monolayers for Resistive Switching Devices Using Machine Learning Potentials and Kinetic Monte Carlo Simulations**
  Developed an equivariant NNP for MoS_2 monolayers with varying S vacancy concentrations; utilized the NNP to drive KMC simulations that model the equilibrium dynamics and vacancy agglomeration into extended defects and the nonequilibrium dynamics of defects for resistive switching devices.

- **Project (4): Prediction of Frequency-Dependent Optical Spectrum for Solid Materials: A Multioutput and Multifidelity Machine Learning Approach**
  Developed multioutput graph neural networks (GNNs) to predict frequency-dependent dielectric functions and absorption coefficients from generic crystal structures, including metals, semiconductors, and insulators, across IR to UV spectra; enhanced model accuracy using multifidelity learning strategies; demonstrated improved learning of solar cell performance parameters through frequency-dependent GNNs with target-specific learning biases.

- **Project (5): Modeling Platinum-Functionalized Graphene for Hydrogen Sensing and Storage Using Machine Learning Potentials**
  Collaborated with NASA Goddard experimentalists to predict crystal structures and growth dynamics of Pt on graphene for advanced gas sensors; employed an equivariant NNP for MD simulations to explore Pt growth modes at varied concentrations; modeled hydrogen adsorption and storage on optimized Pt/graphene structures via MD simulations.

- **Project (6): Experimental and Theoretical Studies of the Surface Oxidation Process of Rare-Earth Tritellurides (RTe_3)**
  Collaborated with experimentalists at Arizona State University to conduct DFT simulations investigating the oxidation of RTe_3 materials; elucidated the oxidation mechanisms and the experimentally observed trends in oxidation resilience across different rare-earth elements.

- **Project (7): A Combined Quantum Monte Carlo (QMC) and DFT Study of the Strain Response and Magnetic Properties of 2D 1T-VSe_2 with Charge Density Wave (CDW)**
  Developed a Python code for spin MC simulations with customizable Hamiltonians; utilized it to study the magnetic thermodynamics and calculate transition temperatures in 1T-VSe_2 monolayers for undistorted and CDW phases under variable strains.

- **Project (8): Quantum Monte Carlo Study of the Multiferroic NiI_2 Monolayer**

Conducted DFT+U noncollinear magnetic calculations for the multiferroic NiI_2 monolayer, analyzed J_1-J_2-J_3 and Dzyaloshinskii-Moriya interaction (DMI) parameters; determined the ground-state spin spiral wavelength and orientation; planning to address deficiencies observed in DFT+U with QMC.

University of Maryland Baltimore County August 2019 – May 2022
Department of Physics
Baltimore, MD, USA
Teaching Assistant

- Led discussions/labs for PHYS 122L, PHYS 121H, PHYS 121, and PHYS 111.

Menoufia University January 2017 – July 2019
Menoufia, Egypt
Teaching Assistant

- Led discussions for classical mechanics, linear algebra, ordinary differential equations, and probability and statistics.

Nagwa, Egypt December 2017 – June 2018
Cairo, Egypt
Physics Content Developer (part-time)

- Developed physics lessons and solutions for the textbook "University Physics OpenStax."

MATERIAL SIMULATION PACKAGES

- DFT: VASP, Quantum ESPRESSO, GPAW, DFTB+, SIESTA/TranSiesta
- MD: LAMMPS, ASE, JAX MD
- Machine Learning Potentials: n2p2, apax, GAP, SchNetPack, MACE, NequIP/Allegro
- Python Materials IDEs: ASE, pymatgen, pyiron
- Cluster Expansion: ATAT, icet
- QMC: QMCPACK

PROGRAMMING SKILLS

GitHub: (link)

- **Programming Languages:** Python, C++, FORTRAN, MATLAB
- **ML/AI Frameworks:** TensorFlow, PyTorch, JAX, PyTorch Geometric, e3nn

PUBLICATIONS

Google Scholar: (link)

1. **A. Ibrahim**, A. Hamze, A. Haldar, Y. Shin, Hybrid Kinetic Monte Carlo and Molecular Dynamics Simulation for Amorphous Boron Nitride Growth Using Machine Learning Potentials **(in preparation)**.

2. **A. Ibrahim**, A. Abdelaziz, M. Sultana, C. Ataca, Modeling Platinum-Functionalized Graphene for Hydrogen Sensing and Storage Using Machine Learning Potentials **(in preparation)**.

3. **A. Ibrahim**, C. Ataca, Modeling Defect Dynamics in MoS_2 Monolayers for Resistive Switching Devices Using Machine Learning Potentials and Kinetic Monte Carlo Simulations **(in preparation)**.

4. D. Wines, **A. Ibrahim**, N. Gudibandla, T. Adel, F. M. Abel, S. Jois, K. Saritas, J. T. Krogel, L. Yin, T. Berlijn, A. T. Hanbicki, G. M. Stephen, A. L. Friedman, S. Krylyuk, A. Davydov, B. Donovan, M. E. Jamer, A. R. Hight Walker, K. Choudhary, F. Tavazza, C. Ataca, A combined Quantum Monte Carlo and DFT study of the strain response and magnetic properties of two-dimensional (2D) 1T-VSe_2 with charge density wave, **arXiv:2409.19082**. (link)

5. **A. Ibrahim**, C. Ataca, Prediction of Frequency-Dependent Optical Spectrum for Solid Materials: A Multioutput and Multifidelity Machine Learning Approach, **ACS Applied Materials & Interfaces**, 16, 31 (2024). (link)

6. **A. Ibrahim**, D. Wines, C. Ataca, Modeling Chemical Exfoliation of Non-van der Waals Chromium Sulfides by Machine Learning Interatomic Potentials and Monte Carlo Simulations, **The Journal of Physical Chemistry C**, 128, 3 (2024)**.** (link)

7. J. Kopaczek, K. Yumigeta, **A. Ibrahim**, M. Y. Sayyad, S. Sinha, R. Sailus, P. Hays, S. T. R. Moosavy, S. Susarla, C. Ataca, R. Kudrawiec, S. Tongay, Experimental and Theoretical Studies of the Surface Oxidation Process of Rare-Earth Tritellurides, **Advanced Electronic Materials,** 9, 5 (2023). (link)

8. G. Chaney, **A. Ibrahim**, F. Ersan, D. Çakır, C. Ataca, Comprehensive Study of Lithium Adsorption and Diffusion on Janus Mo/WXY (X, Y = S, Se, Te) Using First-Principles and Machine Learning Approaches, **ACS Applied Materials & Interfaces**, 13, 30 (2022). (link)

AWARDS

- GDS IMPACT Award for Excellence in Graduate Research, APS (2023).

TALKS AND PRESENTATIONS

1. Modeling Crystal Growth of Amorphous Boron Nitride via Hybrid Kinetic Monte Carlo and Molecular Dynamics using Machine Learning Force Fields, SSI AML, August 2024.
2. DFT+U Study of Magnetic Properties of Multiferroic NiI_2 Monolayers, QMMS workshop, February 2024.
3. Neural network potentials for nonstoichiometric materials: a case study for chromium sulfides $Cr_{(1-x)}S$, AIMS workshop, July 2023.
4. Machine learning modeling of the self-assembly of one-dimensional nanostructures from two-dimensional MoS_2 monolayers with defect and strain engineering, APS, March 2023.
5. Physically informed graph neural networks for prediction of optical properties of solid materials, APS, March 2023.
6. Experimental and theoretical studies of the surface oxidation process of Rare-Earth Tritellurides, QMMS workshop, February 2023.
7. Neural Network Potentials for Nonstoichiometric Materials: a case study for chromium sulfides, APS Mid-Atlantic, December 2022.
8. Machine-learned molecular dynamics modeling of the self-assembly of one-dimensional nanostructures from MoS_2 monolayers with defect engineering, AIMS workshop, July 2022.