# Akram Ibrahim, M.S.

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

## EDUCATION

**University of Maryland Baltimore County** May 2025 (**Expected Graduation**)
**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) Simulations for Amorphous Boron Nitride (aBN) Growth Using Machine Learning Potentials**
  Developed "KMCPACK," a Python package within the Atomic Simulation Environment (ASE) for hybrid KMC/MD simulations: supports lattice-free modeling of bottom-up crystal growth methods like chemical vapor deposition, facilitates the growth of amorphous/crystalline materials with well-defined mechanisms for key KMC events, including sensitive deposition of user-defined precursors, management of high- and low-probability desorption reactions over MD timescales, and enables custom event definition and processing; implemented a neural network potential (NNP) for aBN growth on Si(111) substrate using different precursors and growth temperatures, benchmarking results against TEM experiments to identify structural motifs crucial for aBN 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-Driven Molecular Dynamics and TEM Measurements**
  Collaborated with NASA Goddard experimentalists to study Pt-functionalized graphene gas sensors for planetary missions; trained and deployed an equivariant NNP for MD annealing and minima hopping simulations to predict Pt/graphene crystal structures at tens of nanometers scale under various Pt loadings and deposition rates; analyzed the nucleation and growth dynamics of Pt on graphene; modeled hydrogen reactivity on optimized structures, assessing capture efficiency, dissociation, and recombination rates, to estimate the optimal Pt loading for hydrogen sensing and storage.

- **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 (SpinMCPack) 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): A combined Quantum Monte Carlo and DFT study of magnetic skyrmions in multiferroic $NiI_2$ Monolayers**
  Conducted QMC and DFT+U noncollinear magnetic calculations to explore magnetoelectric interaction parameters in multiferroic $NiI_2$ monolayers; analyzed $J_1$-$J_2$-$J_3$ interactions, magnetic anisotropy, and electric polarization induced by spin spirals; determined the ground-state spin spiral wavelength and orientation; enhanced the Python code (SpinMCPack) to simulate and control magnetic skyrmion formation via external fields; identified transition temperatures for magnetic ordering and skyrmions.

**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, Ovito
- 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. Abdelaziz, M. Sultana, C. Ataca, Modeling Platinum-Functionalized Graphene for Hydrogen Sensing and Storage Using Machine Learning-Driven Molecular Dynamics and TEM Measurements **(in review).**

2. **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)**.

3. **A. Ibrahim**, N. Gudibandla, D. Wines, K. Saritas, C. Ataca, A combined Quantum Monte Carlo and DFT study of magnetic skyrmions in multiferroic $NiI_2$ Monolayers **(in preparation)**.

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

5. 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, Accepted at ACS Nano**. (link)

6. **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)

7. **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), **special issue "Machine Learning in Physical Chemistry Volume 2".** (link)

8. 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)

9. 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, Samsung Semiconductor 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.

## ACADEMIC & INDUSTRIAL REFERENCES

1. Dr. Can Ataca (ataca@umbc.edu)
2. Dr. Yongwoo Shin (yongwoo.s@samsung.com)
3. Dr. Ali Hamze (ali.hamze@samsung.com)