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Machine Learning Approach for the prediction of Structural and Ferroelectric Properties of Two-Dimensional (2D) Halide Perovskite Materials

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Abstract

Two-dimensional (2D) halide perovskites are forthcoming as promising candidates for next-generation ferroelectric and optoelectronic devices. Traditional discovery methods are computationally intensive and slow because they cover a large memory and space. In this study, we used a graph neural network (GNN) framework to more quickly forecast the structural and ferroelectric properties of 2D halide perovskites. Density functional theory (DFT) was used to generate a diverse dataset of polar and non-polar perovskite monolayers, including formation energies, spontaneous polarization, and band gaps. A GNN model that could precisely replicate DFT-level property trends at a fraction of the cost was trained using these DFT-relaxed structures recorded as crystal graphs. To facilitate rapid structural relaxation, a GNN-based interatomic potential was also developed, which identified key polar distortions and showed good agreement with DFT geometries. Some 2D halide perovskites with expected significant out-of-plane polarization and excellent stability are revealed by high-throughput screening throughout a wide A–B–X chemical space.

Keywords
2D Halide Perovskite, Graph Neural Networks (GNNs), Density Functional Theory (DFT), Ferroelectricity

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Biographies
Mahin Muntasir obtained his BS in materials science degree from Khulna University of Engineering and Technology (KUET), Bangladesh. He is a graduate researcher pursuing his M.S. in Applied Optics degree at Delaware State University (DSU). His research focuses on thin-film materials, including rare-earth–doped aluminum nitride (AlN) thin films for ferroelectric applications and advanced microbolometer materials for uncooled infrared detection. He has experience with RF sputtering, device fabrication, materials characterization, and DFT-based computational

modeling. Mahin has worked on optimizing deposition parameters, studying crystallographic behavior, and analyzing electrical and optical responses of functional thin films. His interests include semiconductor device engineering, computational materials science, and advanced thin-film technologies. He aims to pursue a Ph.D. in Materials Science with a focus on electronic and ferroelectric materials. Mahin is committed to developing next-generation materials for sensing and energy applications.

Razia Khan Sharme obtained her BS in materials science degree from Khulna University of Engineering and Technology (KUET), Bangladesh. She is now a master's student in Applied Optics at DSU. Razia works under the supervision of Dr. Mukti Rana, where her research integrates both experimental and simulation approaches to develop transparent conductive coatings for advanced space applications, including GNC LiDAR systems. She completed a research internship at NASA Goddard Space Flight Center, contributing to the development of environmentally friendly, durable anti-reflective thin films. With a background in Materials Science and Engineering, Razia has presented her work at leading national conferences and continues to be recognized for her contributions to the fields of optics and materials science.

Alvee Alam is an undergraduate student in the Department of Electrical, Electronic, and Communication Engineering at the Military Institute of Science and Technology (MIST), Bangladesh. He is currently conducting density functional theory (DFT) simulations on perovskite materials to study their optical, electronic, mechanical, and structural properties. His research interests include computational materials science, semiconductor physics, and advanced functional materials. Along with his academic work, Alvee is passionate about sports and actively enjoys playing various games. He aims to continue developing his skills and contributing to innovative research in electronic and photonic materials.

Dr. Mukti M. Rana earned his B.Sc. in Electrical and Electronic Engineering from KUET, Bangladesh. He completed his M.S. and Ph.D. in Electrical Engineering at The University of Texas at Arlington (UTA). During his graduate studies, he worked as both a teaching assistant and a research assistant. His Ph.D. research focused on RF-sputtered $Ge_xSi_{1-x}O_y$ thin films for uncooled infrared detection. He also designed, fabricated, and tested microbolometers using these materials. After completing his Ph.D., he worked as a postdoctoral research associate on design, fabrication and implementation of sensors for cardiopulmonary resuscitation (CPR) uses. Dr. Rana joined in the Department of Electrical and Computer Engineering of University of South Alabama as an Assistant Professor in 2008. In 2010, he moved to Delaware State University, where he is a Professor of Engineering. His research interests include 2D/3D interfaces, 2D materials, ferroelectric thin films, infrared detectors, and MEMS devices. He has published over 55 papers, holds four U.S. patents, and has received major awards including NASA's Faculty Mentor of the Year (2019).