ABSTRACT & BIO

TITLE: AI-Driven Design of High Entropy Halide Perovskite Alloys

Arun Mannodi-Kanakkithodi[1], Jiaqi Yang[1], Panos Manganaris[1], Maria K.Y. Chan[2], Rishi E. Kumar[3], David P. Fenning[3]

[1]School of Materials Engineering, Purdue University, West Lafayette, IN 47906

[2]Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439

[3]Department of NanoEngineering, University of California San Diego, CA 92093

Halide perovskites with desirable stability, electronic structure, and optical absorption are sought for solar cells, electronic devices, infrared sensors and quantum computing. Compositional manipulation via alloying at cation or anion sites, or via incorporation of point defects and impurities, can help tune their properties. In this work, we develop AI-based frameworks for the on-demand prediction and optimization of the phase stability, band gap, optical absorption spectra, photovoltaic figures of merit, and defect formation energies for a chemical space of ABX_3 halide perovskites with several choices for A, B and X, with mixing allowed at each site. These frameworks are powered by high-throughput density functional theory (DFT) computations, unique encoding of atom-composition-structure (ACS) information, and rigorous training of advanced neural network (NN)-based predictive models and genetic algorithm (GA)-based multi-objective optimization frameworks. Our models scale robustly well to large system sizes as well as varying amounts of mixing of completely new elements at cation or anion sites. Recommendations from combinatorial screening and GA-based design are synergistically coupled with targeted synthesis and characterization, leading to successful validation and discovery of novel halide perovskite compositions for improved performance in solar cells.

Arun Mannodi Kanakkithodi is an assistant professor in Materials Engineering at Purdue University. He received his PhD in Materials Science and Engineering from the University of Connecticut in 2017 and worked as a postdoctoral researcher at the Center for Nanoscale Materials in Argonne National Laboratory from 2017 to 2020. His research involves using first principles computational modeling, machine learning, and materials informatics to drive the design of new materials for energy-relevant applications. He is a resident associate in the Nanoscience and Technology Division at Argonne, a regular attendee, presenter, and organizer at the Materials Research Society (MRS) spring and fall meetings, and a co-organizer of the data science and machine learning workshop series as part of the NSF-funded nanoHUB.org.