Machine Learning Models to Assist Designing Atomic Environments in Semiconductor Heterostructures and Complex Alloys

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ABSTRACT

Following empirical, theoretical, and computational eras of material development, machine learning (ML)-based materials design and discovery research has emerged as the fourth paradigm of materials science. In my research group at the University of Colorado at Boulder, we leverage ML models to design and discover new materials to realize future technologies. Additionally, we discover materials design strategies that will optimize properties of nanoscale materials. In this talk, I will present an overview of activities of my research group, with particular focus on our use of ML models to predict electronic properties of two classes of materials: (1) semiconductor heterostructures and (2) complex multicomponent alloys.

Over the past few decades, semiconductor heterostructures have emerged as key enabling materials for essential technologies, including telecommunication systems, light-emitting diodes, or high-electron-mobility transistors used in high-frequency devices. The heterostructures are strongly affected by the growth processes. It remains a challenge to explore the vast structural parameter space of 'real' heterostructures using first-principles modeling techniques, due to high computational costs. In particular, the calculations of electronic transport coefficients (such as, thermopower or conductivity) require large number of individual energy calculations and computational costs can accrue quickly. In this talk, I will discuss how the use of ML models can assist us in extending the applicability of these *ab initio* techniques to 'real' heterostructures. I will discuss a forward ML-model that can predict the Seebeck coefficients of fabricated semiconductor heterostructures of thickness upto ~12 nm [1]. Additionally, I will present an inverse approach that predicts the atomic-scale features of a given heterostructure that will result in target electronic band structures [2].

In recent years, a new alloying strategy that aimed to stabilize (near) equimolar mixtures of multiple elements by maximizing the configurational entropy has revealed unprecedented opportunities for materials discovery. The alloy mixtures became known as high-entropy materials. The alloys exhibit unprecedented combinations of mechanical and functional properties, even at extreme environments, making them attractive for energy and aerospace applications. The vast compositional space offers enormous possibilities to engineer lattice and electronics structures and tune the properties. However, the `needle in a haystack' scenario puts targeted alloy design to its hardest test: new materials with exceptional properties can hide in practically infinite and vastly unexplored composition space. I will discuss a ML-based approach that can guide the design and discovery process of novel alloys and compounds.

1. A. K. Pimachev and S. Neogi, "First-principles prediction of electronic transport in fabricated semiconductor heterostructures via physics-aware machine learning." *npj Computational Materials*, *7*(1), 93 (2021).
2. A. K. Pimachev and S. Neogi. "Deep Learning Model for Inverse Design of Semiconductor Heterostructures with Desired Electronic Band Structures." arXiv preprint arXiv:2302.00261 (2023).