Implementation of Density Functional Theory (DFT) and Artificial Intelligence (AI) in Indium Tin Oxide (ITO)

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Abstract

Oxide semiconductors, such as indium tin oxide (ITO), are emerging as promising materials for the development of future field-effect transistors (FETs) in three-dimensional integrated circuits (3D ICs). This potential stems from their unique properties, including a low thermal budget, superior FET performance, and scalability. Despite these advantages, several technical challenges remain before their full potential can be realized in practical applications. Among the most pressing issues are material uniformity, interfacial quality, and the comprehensive understanding of the underlying physics that govern these materials.

Currently, Density Functional Theory (DFT) offers high accuracy in modeling atomic interactions, but its application is limited to relatively small systems due to computational constraints. On the other hand, conventional Molecular Dynamics (MD) simulations are capable of handling larger systems but lack the atomic-scale precision required for nuanced insights into material behavior. This research aims to overcome these limitations by integrating artificial intelligence (AI) techniques, specifically deep neural networks, to develop a more sophisticated simulation framework that maintains atomic-scale accuracy in large-scale systems.

In this study, a novel approach that utilizes deep potential training to create a highly accurate force field for indium oxide (In_2O_3) was introduced. Our model accounts for atomic distortions and vacancies, achieving remarkable accuracy in predicting both energy and force. This innovation is particularly advantageous for simulating amorphous and large-scale systems of In2O3, a material critical to the advancement of next-generation semiconductor devices.

Preliminary results from Molecular Dynamics simulations using our deep potential model on a 1 nm thick In_2O_3 slab demonstrate system stability and reliability, providing a solid foundation for further exploration. This approach not only enhances our understanding of the material's properties but also opens new pathways for investigating its potential applications in complex semiconductor architectures.

Looking forward, our research will extend to the incorporation of tin (Sn) doping to explore the behavior and properties of the InSnO complex. This extension will allow for a deeper examination of the amorphous and large-scale system predictions for ITO, thereby expanding our understanding of its application potential in advanced electronic systems.

Keywords - ITO, In_2O_3, AI, Deep Potential MD, DFT, semiconductor devices