

Predicting the Structure and Properties of Inorganic Epitaxial Interfaces

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Epitaxial inorganic interfaces lie at the heart of semiconductor, spintronic, and quantum devices. At an interface between two dissimilar materials (*e.g.*, a ferromagnet and a semiconductor) physical properties and functionalities may arise, which do not exist in any of the isolated constituents in the bulk. The resulting device performance hinges on the electronic and magnetic properties of the interface, as well as on its quality. As devices become increasingly smaller, precise control over interface structure becomes increasingly critical. At the same time, the configuration space of possible inorganic interfaces is vast and largely underexplored, owing to the almost infinite number of ways different materials can be combined to form interfaces. The experiments required to fabricate high-quality defect-free interfaces and devices are costly and time consuming. Therefore, it is unfeasible to explore the space of possible structures and compositions by experimental means alone. Computer simulations may significantly accelerate the discovery and design of new inorganic interfaces with desirable properties.

To predict the structure of domain-matched epitaxial interfaces, we have developed the Ogre code [1]. Ogre starts by performing “lattice matching” to identify all possible domain-matched commensurate interfaces within the range of user-defined Miller indices, maximum strain, and maximum area. For each orientation, Ogre constructs interface structures by identifying and combining all possible surface terminations of the two materials. Subsequently, for each interface, Ogre performs “surface matching” to identify the best in-plane registry and interfacial distance between the two materials. Finally, all candidate interfaces are ranked by stability.

To study the electronic properties of interfaces we use density functional theory (DFT). Within DFT, the many-body interactions between electrons are described by approximate exchange-correlation functionals. The accuracy of the results hinges on an appropriate choice of functional. We have developed a method of machine learning the Hubbard U correction added to a DFT functional by Bayesian optimization (BO) [2]. The DFT+U(BO) method balances accuracy with computational cost, enabling unprecedented simulations of large surface and interface models of interest for applications in quantum computing. For example, we have used DFT+U(BO) to assess candidate materials for tunnel barriers at semiconductor/ superconductor interfaces [3,4].

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