Structure prediction of epitaxial inorganic interfaces by lattice and surface matching with Ogre

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Abstract

We present a new version of the Ogre open source Python package with the capability to perform structure prediction of epitaxial inorganic interfaces by lattice and surface matching. In the lattice matching step, a scan over combinations of substrate and film Miller indices is performed to identify the domain-matched interfaces with the lowest mismatch. Subsequently, surface matching is conducted by Bayesian optimization to find the optimal interfacial distance and in-plane registry between the substrate and the film. The optimized interfaces are pre-ranked using a score function based on the similarity of the atomic environment at the interface to the bulk environment.. The application of Ogre is demonstrated for two interfaces of interest for quantum computing and spintronics, Al/InAs and Fe/InSb.

Introduction to interface structure prediction

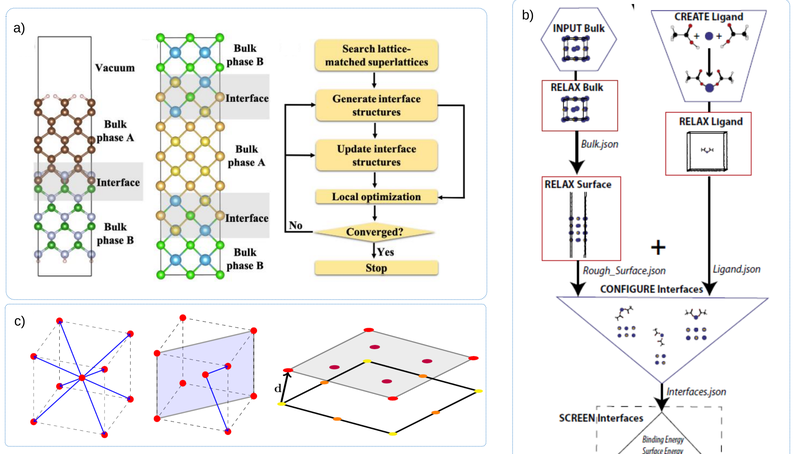

Fig 1. Recent trends toward structure prediction of interfacial systems. a) Combining a search algorithm with efficient calculation method b) High throughput first principle calculation of possible interfaces c) fast screen of latticed matched structures using an effective score function

Methods

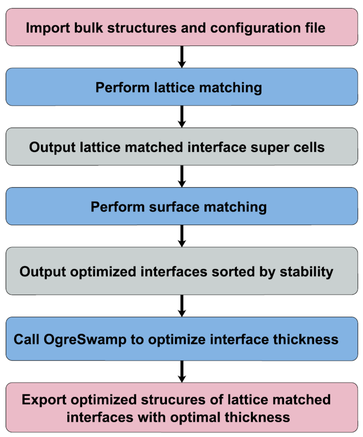

Fig 2. Workflow of interface structure prediction with Ogre. The pink boxes represent code inputs and outputs. The blue boxes represent different code modules. The gray boxes show module outputs that serve as inputs of the subsequent module.

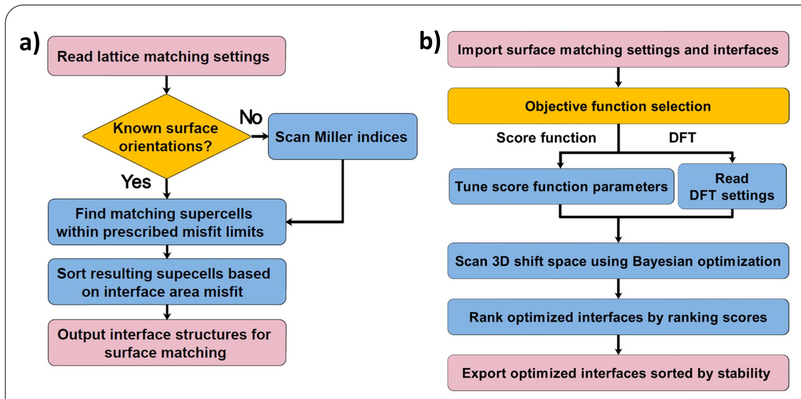

Fig 3. A) Workflow of interface structure prediction with Ogre. B) The workflow of surface matching in Ogre. The pink boxes represent code inputs and outputs. The blue boxes represent different code modules. The gray boxes show module outputs that serve as inputs of the subsequent module.

Results and discussion

$$S = (1+\bar{O})^2 + c\bar{E}, \quad \bar{O} = \frac{V_O}{\sum_{atoms} V_{at}}, \quad \bar{E} = \frac{V_E}{V_{cell}}$$

$$R_M = \frac{\rho}{1+\rho} \times D_{MX}, \rho = \sqrt[3]{\frac{H_{V,M}}{H_{V,X}}}, R = \left|\bar{O}_{int}^{film} - \bar{O}_{slab}^{film}\right| + \left|\bar{O}_{int}^{sub} - \bar{O}_{slab}^{sub}\right|$$

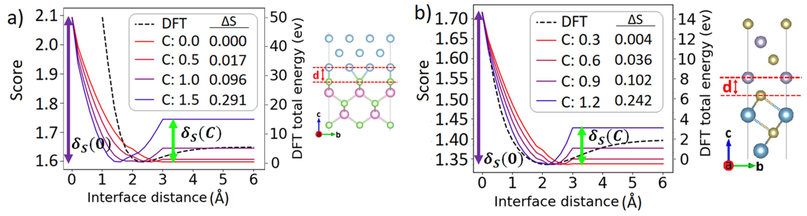

Fig 4. Performance of the geometric score function for determining the interfacial distance: The score obtained with different values of c as a function of the interfacial distance in the z direction compared to the DFT total energy curves for (a) the Al(100)/InAs(100) interface and (b) the SnTe(111)/CaTe(111) interface. The DFT energy minimum is referenced to zero.

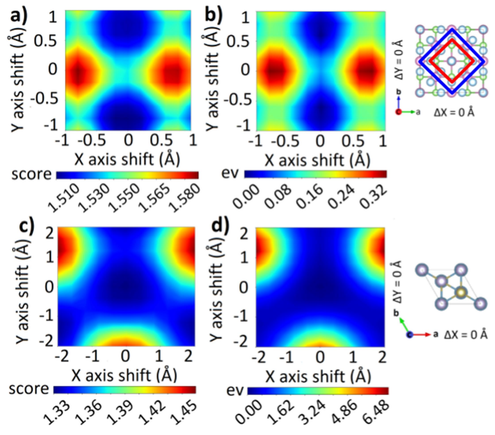

Fig 5. Performance of the geometric score function for the registry in the xy plane: (a) Score function contour plot compared to (b) the DFT potential energy surface at a fixed interfacial distance of 2.2 A for the Al(100)/InAs(100) interface. (c) Score function contour plot compared to (d) the DFT potential energy surface at a fixed interfacial distance of 2.0 A for the SnTe(111)/CaTe(111) interface. The DFT energy minimum is referenced to zero.

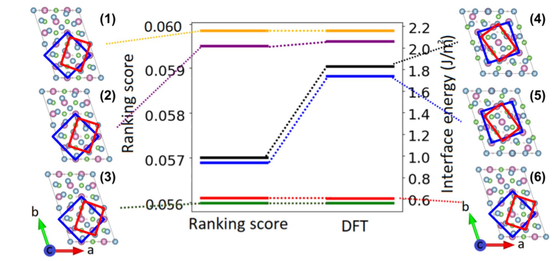

Fig 6. The ranking score compared with DFT interface energies for the six most stable structures of the Al(011)/InAs(100) interface. The ranking score correctly reproduces the order of stability obtained from DFT.

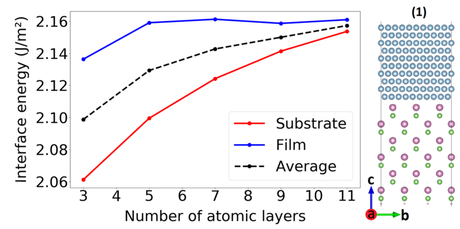

Fig 7. Interface energy convergence plots for an Al(111)/InAs(001) interface

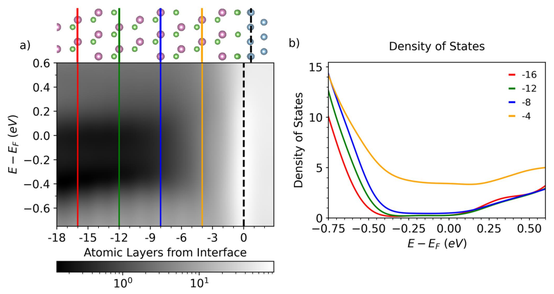

Fig 8. Electronic structure of the most stable Al(111)/InAs(111) interface structure: (a) the density of states as a function of distance from the interface with the interface structure illustrated on top. Al, As, and In atoms are colored in light blue, green, and pink, respectively. (b) The local density of states of InAs at 4, 8, 12, and 16 layers from the interface, indicated in (a) by vertical lines in the same colors.

Conclusion

Ogre may advance understanding of the structure and properties of epitaxial inorganic interfaces, as well as the computational design and discovery of new interfaces by being used to:

- **Interpret the results of experiments conducted on epitaxial inorganic interfaces by identifying the most likely interface configurations and correlating the structures with the observed electronic properties and/or spectroscopic signatures.**
- **Predict the structure and properties of putative interfaces and guide synthesis efforts in promising directions.**
- **Get incorporated into an automated materials discovery workflow.**

References

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