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Relevant publications:

Interface AIRSS: “Predicting interface structures: From SrTiO_3 to graphene”,
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AIRSS: “High-Pressure Phases of Silane”,
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CASTEP: “First principles methods using CASTEP”,
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and M. C. Payne, Z. Kristallogr. 220, 567 (2005).

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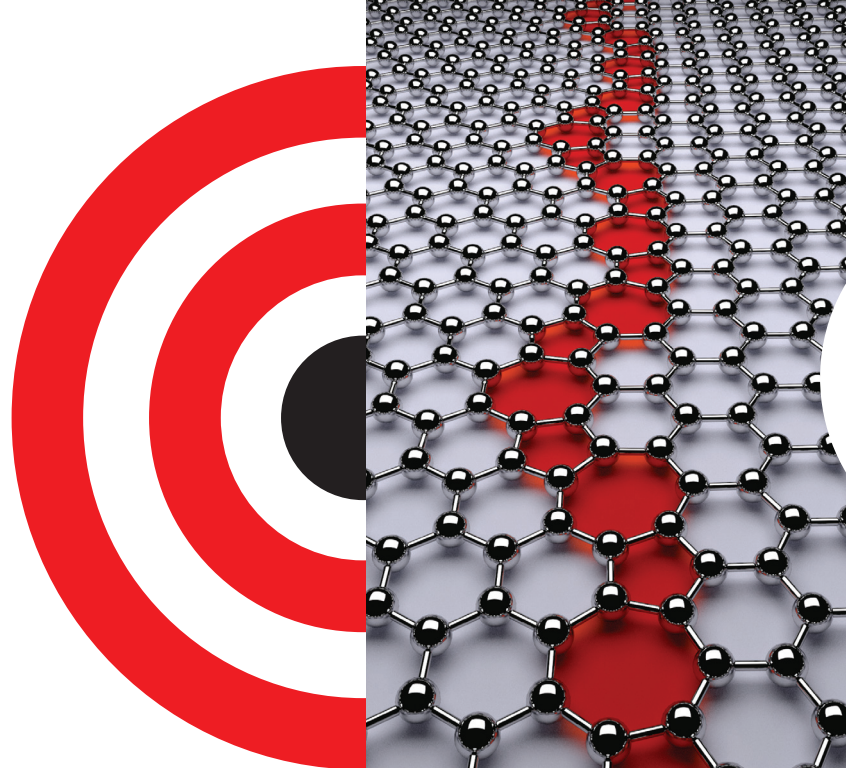
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The Case Study Series

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INTERFACE STRUCTURE PREDICTION FOR FUTURE TECHNOLOGIES - A ROUTE TO “INTERFACES BY DESIGN”

We have developed a general first-principles approach to predict the crystal structure of interfaces in materials, a technique that represents a major step towards computationally developing materials with specially designed interfaces.

“Interfaces by Design” has the potential to bring crucial advances to the understanding and design of interfaces with unique electronic, optical and mechanical properties in future materials. This may lead to novel technologies in many sectors of industry, in particular the microelectronics and optoelectronics industry.

A number of international initiatives have been set up with the aim of employing computational techniques to shorten the time and decrease the cost of the R&D cycle to commercialisation, with Materials Discovery and Materials by Design forming an integral part. Most approaches so far have however focused primarily on finding and classifying bulk materials and their properties, that is materials in their ideal crystal structure, without defects and without internal interfaces or interfaces to other materials.

However, materials in nature and most devices are usually not ideal, perfectly crystalline materials, but instead are often polycrystalline. Two-dimensional graphene, for instance, is often considered as an ideal perfectly crystalline 2D material, while it is predominantly grown as a polycrystalline material. That means that it really consists of regions of perfect crystalline shape (“grains”) that are rotated with respect to neighbouring ideal regions. The crystal structure of these interface regions (or “grain boundaries”) can significantly affect the electronic, optical and mechanical properties of polycrystalline materials.

Similarly, most state-of-the-art devices rely on so-called heterostructures, where interfaces are formed between two different materials. The device properties often crucially depend on the exact nature of these interfaces. Heterostructures are omnipresent in the microelectronics and optoelectronics industry, forming the basis of most of today's high-tech devices, such as transistors in computers and smartphones, and the optical components in displays.



Though such polycrystalline and heterostructure materials can today be routinely grown experimentally, for many of these it is not easy to determine the atomic structures experimentally, making understanding their properties and the underlying physics that govern them a slow, difficult and often expensive task.

Using simulations, we can gain a better understanding of the physics of grain boundaries and heterostructure interfaces, which in turn is crucial for the development of better and novel devices. The fundamental bottleneck here is however first finding the exact crystal structures involved.

Our ability to find the low energy, stable atomic structures of interfaces – that is, the structures most likely to be found in the real world – is still very limited and so far largely overlooked in the context of most approaches to Materials by Design.

The key achievement in our work has been to develop an approach to predict the crystal structures of interfaces.

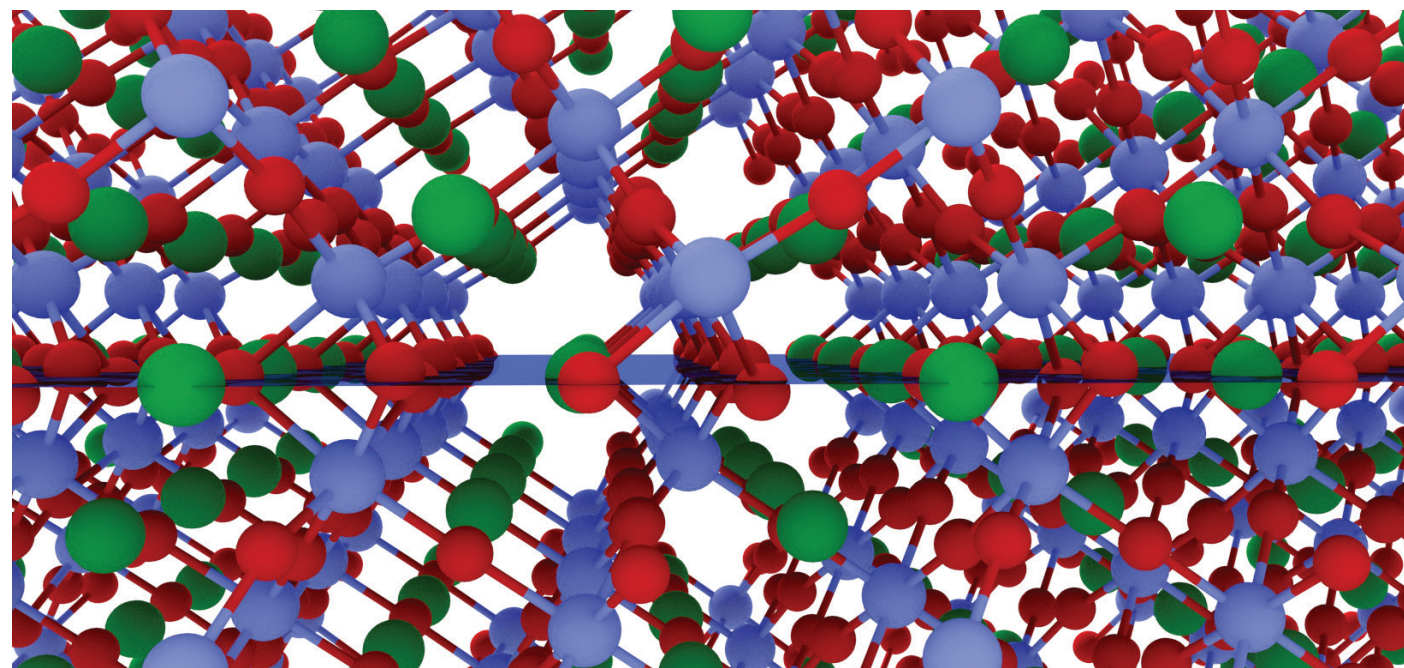
This is based on the ab initio random structure searching (AIRSS) approach, which has been successfully used for bulk structure prediction in the past. It is implemented to employ the CASTEP code, and by using the availability of greater computational power from ARCHER we have now shown that it is feasible to apply this technique to systems with large interfaces.

Due to the large number of atoms involved in interface structure prediction, the computational cost is significantly greater than for more conventional bulk-type structure prediction. The computational resources available from ARCHER, and previously HECToR, enabled this work to be accomplished. It would not have been feasible to perform many of these calculations on local clusters.

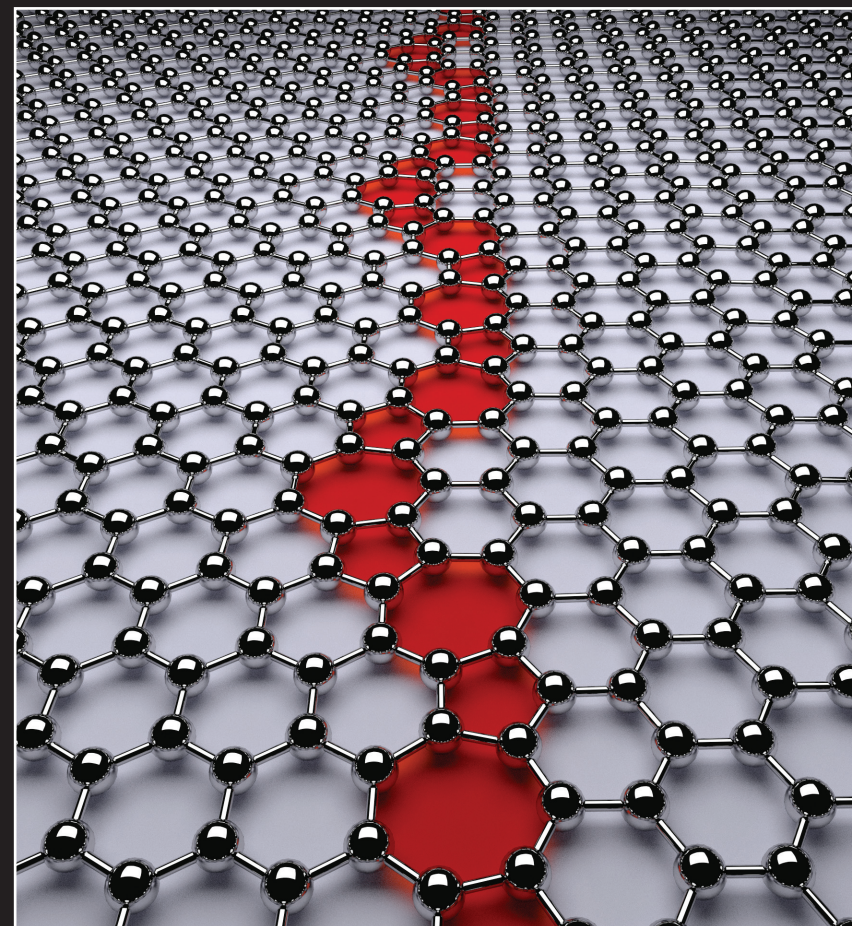
In particular, we have studied grain boundaries in two structurally and chemically very different materials, graphene and strontium titanate, and found new low energy structures for both systems. Both materials are important to the microelectronics industry, but more importantly each also represents a larger class of materials, and a better understanding of the crystal structure and properties of their grain boundaries has the potential to make significant long-term impact in this and other industry sectors.

Our method is not limited to these particular elements and indeed one of its strengths lies in its generality – it can be applied to a wide variety of materials. At present our approach is designed to be employed in synergy with experiments. Experimental results allow us to introduce constraints to our calculations, which reduces the otherwise enormous search space associated with interface structure prediction. It is envisioned that with ever increasing computational resources, ever more complex systems can be addressed and studied purely computationally, thereby leading to a stand-alone purely theoretical approach to “Interfaces by Design”.

This has the potential to bring significant savings to industry and improvements to a wide range of technologies.

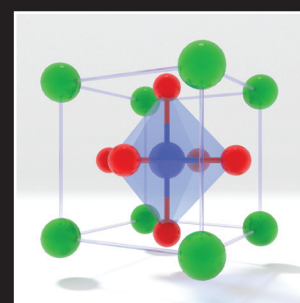


SrTiO₃ symmetric tilt grain boundary. The blue transparent region marks the grain boundary plane, separating two tilted regions of SrTiO₃. Blue, green and red spheres represent titanium, strontium and oxygen atoms, respectively.



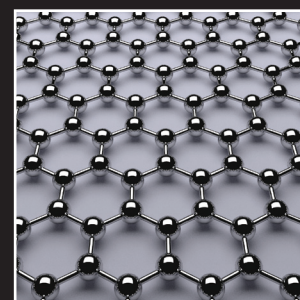
Graphene grain boundary

Graphene grain boundary structure between armchair and zigzag graphene regions. The red transparent region marks the interface between the two grains, forming a continuous chain of pentagons and heptagons in the otherwise pristine graphene.



Strontium Titanate (SrTiO₃)

is a transition metal oxide that already finds applications in a wide range of technologies in the microelectronics industry: capacitors, thermistors and varistors, to name a few. It is also considered as a possible candidate material in next generation metal oxide semiconductor field effect transistors (MOSFET) – the transistors in computer processors. Transition metal oxides in general have numerous applications, ranging from optical applications, such as solar cells and optical displays, to applications in microelectronics, as well as coatings and catalysts.



Graphene

is a two-dimensional material consisting of a hexagonal lattice of carbon atoms, and based on a single layer of graphite. It is the prototypical example of a large range of two-dimensional materials, with often very unique properties. To date the number of commercial products available using graphene is limited, but it has huge promise in future application in the microelectronics industry.