Theoretical Spectroscopy of Nanomaterials

A highly-motivated PhD candidate is sought to join the group of Dr Nicholas Hine, who is joining the Physics Department at the University of Warwick in 2015. The proposed research will involve using computational modelling to understand the properties of nanomaterials, namely materials with complex structure at the nanometre scale which determines their function. State-of-the-art quantum mechanical methods based on linear-scaling density functional theory now allow us to accurately model the electronic structure of systems as large as whole nanocrystals, heterostructure interfaces, proteins, molecular crystals, and defects in semiconductors. This allows us to understand their fundamental physics and make precise predictions of their properties.

Recent work has focussed on simulating the results of advanced techniques in experimental spectroscopy, such as EELS and XAS: in this project we seek to extend this to intersect with experimental work at Warwick to underpin the development of new materials and devices in active areas such as photovoltaics and photocatalysis, quantum biology, and quantum information processing.

Along with other academics at Cambridge, Imperial and Southampton, Nicholas Hine is an author of the [ONETEP Linear-Scaling Density Functional Theory (DFT) Code](). The computational effort involved in traditional approaches to DFT scales cubically with system size, preventing calculations of more than a few thousand atoms. Linear-Scaling approaches to DFT use methods based on local orbitals to avoid the cubic scaling steps and thus scale linearly with system size.

The student should be keen to use computational simulations and High-Performance Computing to understand fundamental properties of materials. A strong background in physics, chemistry or materials and good mathematical skills are vital, and some knowledge of coding and numerical methods is desirable. This project will have close connections to experimental work at Warwick, and with ongoing methodological development at Cambridge, London and Southampton as part of the wider ONETEP project. Several different application areas are possible:

1) Excited States of defects in Diamond Nanocrystals

Nanocrystals of diamond have many possible applications in areas such as quantum information processing, nanophotonics, and sensing: in particular, their defects, such as the nitrogen vacancy (NV) centre. This application would involve using Linear-Scaling DFT to model whole nanocrystals containing defects, to understand how their excited states depend on size, shape, surfaces, and the many other degrees of freedom available to nanocrystals.

2) Understanding van der Waals heterostructures

Layered materials such as graphene, MoS_2 and WSe_2 have numerous exciting properties, but we are reaching the point where we already understand all the fundamental physics of their monolayer forms. However, these materials can be combined simply by stacking them on top of each other, enabling many new combinations of properties, of importance in optoelectronics, low-power electronics, and photocatalysis. We can use LS-DFT to model interfaces and nano-flakes of such materials, to elucidate how their properties depend on angular alignment and edge termination.

3) First-principles Thermodynamics of defects in semiconductors and complex oxides

Individual point defects in crystals are at the heart of important materials properties such as electrical and ionic conductivity, oxide scale growth, and many more:. Accurate calculations of defect formation energies allow us to predict the concentrations of such defects from first principles, allowing us to suggest systematic design rules to improve high-performance materials.