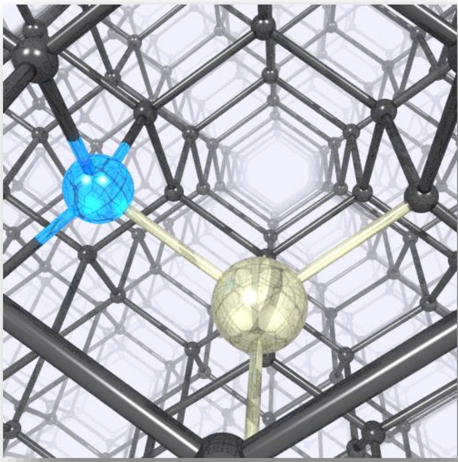
First principles modelling of the excited state & simulated spectroscopy (Newcastle University)

About the project

Electrons move in solids in a fashion dictated by the laws of quantum-mechanics, so that everyday observations, such as the colour of a crystalline material, cannot be predicted or explained without grasping the wave-like nature of the electrons involved. However, the wave functions of electrons cannot easily be seen **directly**, and it is a key role of computational science to provide much of the detail.



Using computers to solve from first principles the equations that govern the interactions between, for example, the light and matter, is not trivial and requires the use of both sophisticated algorithms and lots of time on parallel-computing systems.

It is of course crucial that the quantum-mechanical modelling is directly relevant to observations in experiment, both quantitatively and qualitatively, but this is an extremely challenging problem. A key example is the case of colour centres in diamond (microscopic, nano-scale defects that give the diamonds colour). For example, the "NV" centre can be electrically charged, has a variety of magnetic properties, and is at the heart of diamond in quantum-computing, colour-centre lasers and single-photon sources used in quantum-encryption. The optical and magnetic properties of this colour centre depend upon the electrons in a complicated, many-body way. In the PhD project, defects, such as NV, are to be modelled using the in-house developed density-functional-theory software, with key objectives in both determining the origins of observed phenomena from experiment, and making predictions of which arrangements of atoms and electrons will provide those properties sought after for a wide range of scientific and technological reasons.

The PhD project, as part of the Diamond Science and Technology Centre for Doctoral Training, is to be conducted in Newcastle University, but in the first year, as part of the MSc year, you will gain experimental experience in two mini-projects in Physics in Warwick University and in the Strathclyde Institute of Photonics. Through these contacts both an appreciation of the challenges in obtaining the experimental data and of the unresolved colour-centre structures will be built, and these links will be maintained to ensure that the modelling and experiment continue to inform one another.

Contacts

Applicants with a good bachelors or a master's degree in the physical sciences (physics, chemistry, engineering, materials) are encouraged to contact Prof Patrick Briddon at patrick.briddon@ncl.ac.uk or Dr Jon Goss at jonathan.goss@ncl.ac.uk. The position consists of a 1 year MSc in Warwick University, followed 3 years in Newcastle University. Details of the programme offered through the Centre for Doctoral Training, including the taught element in the first year and the available funding, can be found online.

About the location of the PhD project

Newcastle University traces its origins back to the College of Medicine and the College of Physical Sciences founded in the 1800s, and is one of the 24 Russel Group of research-intensive UK Universities. The 50-acre main site is unusual in being a city-centre campus (you can take a virtual tour online), with the obvious advantages of being just minutes away from the heart of the city. In addition to being a top 10 UK Universities for student experience, we are one of only 9 UK Universities with a Silver Athena SWAN award, underlining the embedding of the diversity and equality agenda throughout our institution.

Lots of additional information about Newcastle University, the City and the region can be found online.

The project supervision will be led by Jon Goss (Senior Lecturer in Physics and Electronic Engineering), who has been working and publishing in the field of QM-modelling of condensed matter problems for 22 years, and co-supervised by Patrick Briddon (Professor of Computational Physics), who has developed the research software at the heart of the research activity. Both supervisors are in the Materials Modelling Group, which lies within the Emerging Technologies and Materials division of the School of Electrical and Electronic Engineering in Newcastle University. The Materials Modelling Group is made up from three academic staff and currently 9 post-graduate and doctoral researchers at various stages.