Project Title: Mechanisms of defect processes in 2D quantum devices

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Project Description:

Point defect qubits in semiconductors have demonstrated their outstanding capabilities for high spatial resolution. 2D hexagonal boron nitride (hBN) hosting point defect qubits have recently opened up new horizons for quantum sensing by implementing sensing foils. For example, negatively charged boron vacancies (V_B^-) in hBN are proposed as atomic scale sensors for temperature, magnetic fields and externally applied pressure. These applications are possible due to the high-spin triplet ground state and bright spin-dependent photoluminescence attributed to V_B^-. Defects are also considered as prospective candidates for quantum computation and are responsible for new modes of device operation, such as neuromorphic systems.

This PhD project will use computational modelling to predict properties of other defects in hBN and other 2D materials for quantum sensing. This will include using the existing and developing novel methods for modelling the structure and properties of defects in 2D heterostructures using atomistic modelling, Density Functional Theory (DFT) and Machine Learning. The project will use large-scale DFT and classical simulations to explore the role of intrinsic defects and impurities in performance of 2D-materials based electronic devices and to develop new modes of their operation. You will learn how to use computer modelling to solve fundamental problems of real impact for design and technology of electronic devices in collaboration with experimental colleagues.

The PhD training and research will be carried out in the group of Prof. Alexander Shluger https://www.ucl.ac.uk/condensed-matter-material-physics/alex-shluger-group in the Department of Physics and Astronomy and LCN. The group is one of the world leaders in computational modelling of defects in insulators and 2D heterostructures underpinning the performance and reliability of electronic devices.

We are looking for a highly motivated candidate with a top-level MSci degree or equivalent in Chemistry, Physics, or Materials. Undergraduate knowledge of Quantum Physics and Solid State Physics is essential. You should enjoy coding and be keen to push the boundaries of machine learning and artificial intelligence in materials applications.