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Materials research within the Excalibur Project: Is it time to exploit Quantum Computers?

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Exascale computing is coming and given the large anticipated power consumption it is prudent to first ensure both the users and the software are exascale ready before investing in the hardware. The Excalibur Project is UK's response to this challenge, which funds a range of hardware and software projects and train the next generation of Research Software Engineers. One of these funded Excalibur projects is called QEVEC, which seeks to determine whether quantum computers could potentially be employed as accelerators for classical HPC. Part of the QEVEC project has targeted the use of D-wave annealers (quantum computers) to tackle problems, in the field of computational chemistry and materials science, that are intractable on classical computers.

In this talk, I will show how the relative energy of defective graphene structures can be calculated by using a quantum annealer. This simple system is used to guide the audience through the steps needed to translate a chemical structure (a set of atoms) and energy model to a representation that can be implemented on quantum annealers (a set of qubits). I discuss in detail how different energy contributions can be included in the model and what their effect is on the final result. The code used to run the simulation on D-Wave quantum annealers is made available as a Jupyter Notebook - more details can be found in our recent publication. The first part of this talk is designed to be a quick-start guide for the computational chemists interested in running their first quantum annealing simulations. The methodology outlined in this talk represents the foundation for simulating more complex systems, such as solid solutions and disordered systems, which I will go on to discuss and show latest results for three different solid solutions, to demonstrate the versatility of our developed method. Each system has interesting technological applications: N-doped graphene in catalysis and energy materials, $Al_\delta Ga_{1-\delta}N$ in optoelectronics and $Mo_\delta W_{1-\delta}$ used as structural components in nuclear and rocket systems because of their high high-temperature strength, high melting point, and good corrosion resistance. Time permitting, I will also present an overview of the Excalibur PAX-HPC project.

Student or Postdoc?

No. Not a student nor Postdoc.

Primary authors: Prof. WOODLEY, Scott (UCL); Dr CAMINO, Bruno (UCL); Dr BUCKERIDGE, John (LSBU); Prof. WARBURTON, Paul (LCN); Dr SOKOL, Alexey (UCL); Dr JEE, Woongkyu (UCL); Prof. CATLOW, Richard (UCL); Dr KENDON, Vivian (Univeristy of Strathclyde)

Presenter: Prof. WOODLEY, Scott (UCL)

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