Exploiting the D-Wave QC for

Exploring Energy Landscapes and Computing Thermodynamical Properties of Materials

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There is already much work on variational quantum eigensolvers (VQE), a type of hybrid quantum-classical algorithm being developed across materials and chemistry simulations; any advantages therein will be realised through already funded projects. However, there are other proposed quantum algorithms that have been less explored but promise potentially larger gains. We will tackle two of these in settings that will readily generalise to other problems: electronic structure calculations that form the basis of Density Functional Theory (DFT) codes such as CASTEP, and solid solutions, an important but hard problem of sampling all possible cation and/or anion ordering on a defined lattice.

Solid solutions are combinations of materials within a single crystal structure, for example, with a simple form A_xB_{1-x}, where $0 \leq x \leq 1$. Such combinations are crucial in catalysis, energy materials and in semi-conductor band structure engineering. In the latter, they are used to realise device applications including laser diodes, LEDs and transistors. Knowledge of the relative proportions of each material that can be incorporated in the solid solution, as well as the distribution of atoms on the crystal sites, is critical for successful device design. For example, in the solid solutions $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$, the quantity x controls the band alignment and hence carrier confinement within semiconductor layers, while the distribution of Al, Ga or In on cation sites in the crystal lattice influences the built-in electric field, which strongly affects carrier recombination rates and hence optical device efficiencies. The aim is to predict the properties of solid solutions as function of temperature, pressure, and chemical potentials. Modelling solid solutions using classical techniques is highly challenging, as a brute force sampling of the phase space is required to predict solubility and atomic distributions under defined thermodynamic conditions. The problem could, however, be tackled with a quantum annealing algorithm, where individual sampling of the phase space would no longer be required, saving considerable computational cost. The relevant interactions can be mapped to an Ising model Hamiltonian, which could be simulated by a quantum annealer such as the D-Wave System. Indeed, a very recent simulation involving defects in graphene, a 2D two-component system, has been demonstrated [1] and we have created a tutorial paper on this [2]. It is crucial to extend such an approach to more complex systems. The 2D MXene solid solution $MoS_{2x}Se_{2-2x}$, of interest for its unusual physical properties and potential applications in catalysis, provides an ideal initial test case. The challenge is due to the increased number of atom types; problems caused by long-range interactions are reduced as the anions have the same charge. Subsequent modelling of the 3D $Al_xGa_{1-x}N$ semi-conductor solid solution, crucial for optoelectronic devices, would prove a step-change in materials modelling capability of quantum systems. 3D systems are more challenging, due to the increased connectivity, but feasible within the timeframe of this proposal. Exploiting D-wave QCs for predicting the structure of materials is a hot topic [3] and we are keen to lead in their applications to problems involving solid solutions.

Initial Objectives: to make a rapid start in this project by first reproducing the results in our tutorial paper [2] and our subsequent technical paper on obtaining thermodynamical properties [4].

The named supervisors are investigators of a significant UK initiative – the Excalibur project [5,6] – that aims to ready the UK for the arrival of exascale computing.

[1] https://doi.org/10.1039/D0CP04037A; [2] https://doi.org/10.1063/5.0151346;
[3] https://doi.org/10.1038/s41586-023-06071-y; [4] Submitted (2024) – a draft of this paper can be made available upon request; [5] https://excalibur.ac.uk/; [5] https://excalibur.ac.uk/projects/qevec/