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A new approach on a D-wave for obtaining thermodynamic properties of a solid solution.

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Alloys, solid solutions, and heavily doped systems, where compositional variation of a multi-component system produces enhanced physical and chemical properties, are critical for key technologies including energy generation and conversion, catalysis, optoelectronics, and smart buildings. However, the simulation of such disordered materials to predict their properties remains an outstanding challenge, even when crystallinity is assumed to be maintained. As x increases in the binary solid solution X(1-x)Yx, there is a "combinatorial explosion" resulting from the fractional occupancy of the sites in the crystallographic unit cell, so that the computation of the energy of all possible combinations becomes intractable. In this talk I will present our latest efforts to exploit the D-wave hardware to extract thermodynamical properties for a solid solution, demonstrated using three different types of materials. The approach developed avoids the poor scaling sometimes experienced when using a QUBO model.
If I have time, I will also present work where we have exploited more traditional computer resources to compute the free energy for charging the cathode of a lithium ion battery.

Student or Postdoc?

Email address

Co-Authors

CHPC User

No

CHPC Research Programme

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Primary authors: Prof. WOODLEY, Scott (UCL); Dr CAMINO, Bruno (UCL)

Presenter: Prof. WOODLEY, Scott (UCL)

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