Determining the thermodynamics of disorder at the nanoscale using quantum computing

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Abstract

Materials that contain disorder at the nanoscale — including alloys, solid solutions, and doped systems — are crucial to technologies such as energy storage, electronics and catalysis. Accurately predicting their properties remains a significant computational challenge due to the vast number of possible atomic configurations that need to be explored in any realistic model. Classical optimisation methods, such as simulated annealing, are routinely applied to this problem, but these approaches spend computational effort exploring high-energy states that are not thermodynamically relevant. We present a novel scalable and accurate method that uses quantum annealing to efficiently sample low-energy configurations in disordered systems. This approach incorporates temperature effects and supports large supercells, generating Boltzmann-like distributions that reflect realistic thermodynamic behaviour. A key feature of the approach is the use of chemical potential to continuously tune the composition of materials, ensuring that the resulting energy Hamiltonians are compatible with current quantum annealing hardware. We demonstrate the efficacy of the method by predicting the band gap bowing in $Al_{1-x}Ga_xN$ and bulk modulus variations in $Ta_{1-x}W_x$, finding excellent agreement with experimental data [1]. Ongoing work explores the extension of this framework to broader classes of disordered systems.

References

[1] Bruno Camino, John Buckeridge, Nicholas Chancellor, C Richard A Catlow, Anna Maria Ferrari, Paul A Warburton, Alexey A Sokol and Scott M Woodley, Science Advances, 23 (2025) adt7156

Figures

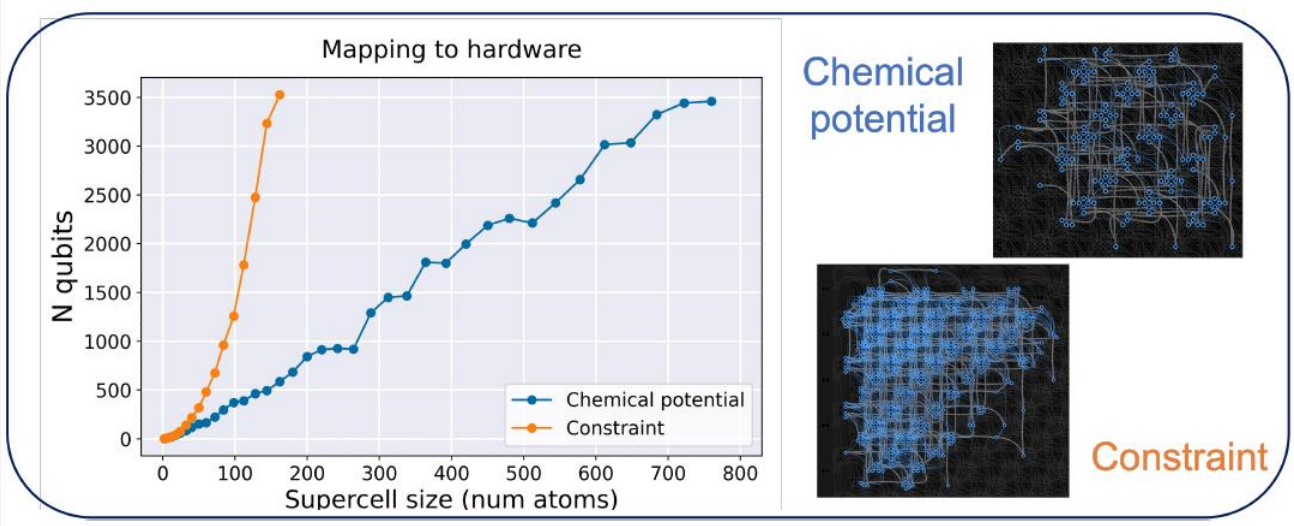

Figure 1: Demonstration of improved scaling with the chemical potential approach to modelling alloys.