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Modeling order-disorder phase transitions with a quantum annealer

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Quantum annealers have grown in complexity to the point that devices with few thousand qubits are approaching capacities to tackle material science problems. Starting from a representation of crystal structures in terms of networks, we develop models of order-disorder phase transitions for two prototypical classes of materials (entropy stabilized alloys and perovskites) that are directly implementable on the D-Wave devices. Cost functions are built to encode the ordered phase, while disordered phases appear as excited states in the spectrum of the classical Ising Hamiltonian, which accounts for the competing interactions in the material. Taking advantage of the statistical nature of the quantum annealing, we explore the energy landscape and generate all the structural models for each step of the order-disorder phenomenon. Besides providing a correct description in terms of critical temperatures, our model allows us to access a wide range of structural models, overcoming some limitations of classical methods.

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