Contribution ID: **14** Type: **not specified**

D-Wave as a generator of structural models for prototypical problems in materials science

Thursday, 7 April 2022 14:45 (45 minutes)

The promise of quantum computing is to provide new methods to unveil the physics of molecules and materials that has been inaccessible to the conventional numerical modeling. Over the past few years, quantum annealers have grown in complexity to the point that the computation of molecular energies has become a feasible application. Whilst typical approaches use quantum annealers to extract the ground state solution of an optimization problem, we suggest a new application as generator of structural models for disordered materials, where disorder appears from the competition between the different degrees of freedom. Starting from the representation of the crystal in terms of network, we map the relevant interactions into Ising Hamiltonians and encode the disordered phases in the excited states spectrum of the target Hamiltonian. In our approach the quantum annealer is used to explore the energy surfaces and to identify stable and metastable phases of prototypical disordered materials.

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Session Classification: Physics of Matter / Quantum