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

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A tool capable to efficiently generate realistic structural models of disordered systems has been a goal of material science for many years. We show the feasibility of quantum annealing in exploring the energy landscape of materials that deviate from the ideal crystalline phase, specifically vacancy defects in graphene and disordered silicon. By mapping the competing interactions onto quadratic unconstrained binary optimization problems (QUBO), our approach guarantees access to all the arrangements of the multiple defects on the graphene sheet respecting the relative formation energies. In the case of silicon a large portion of the structural models with an increasing disorder is encoded in the low energy spectrum of the QUBO formulation and detected in the annealing process. Our approach reproduces known results and provides a stepping-stone towards applications of quantum annealing to more complex problems of physical-chemical interest.

Presenter: CARNEVALI, Virginia (Central Michigan University)

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