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D-Wave as a generator of structural models for order-disorder transitions in materials science

Rosa Di Felice

Departments of Physics and Astronomy and Quantitative and Computational Biology, University of Southern California, Los Angeles, USA

CNR-NANO Modena, Italy

difelice@usc.edu

With: Virginia Carnevali and Marco Fornari at Central Michigan University, Ilaria Siloi at USC

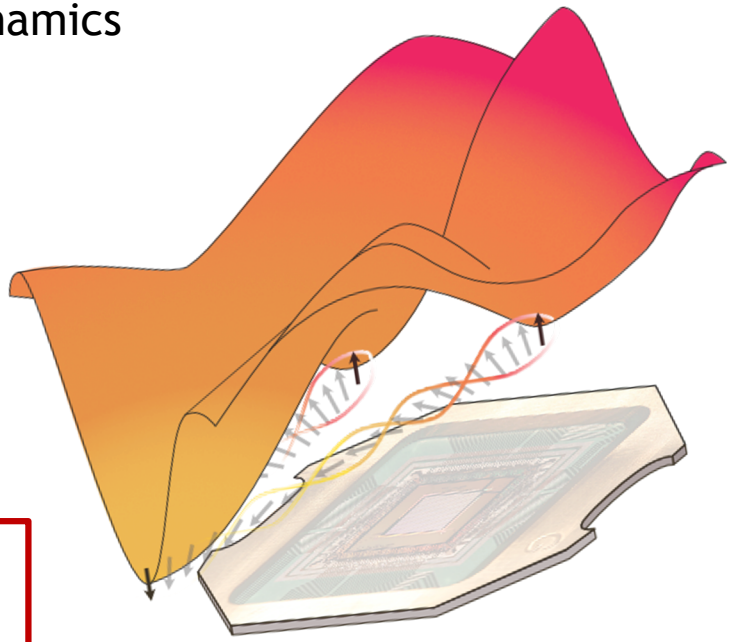
Prologue

The progress of computer power and integration and parallelization has greatly boosted discoveries in biology, chemistry, materials science and big-data fields of research

Can the same disciplines/fields take even more advantage from quantum computers?

Outline

- Introduction: quantum annealing and materials thermodynamics
- QUBO formulations for materials phases and results
  - Melting: amorphous silicon
  - Entropy stabilization: high-entropy alloys
  - Order-disorder transitions: perovskites
- Summary



The generation of structural models for real materials requires the exploration of the Born-Oppenheimer surface, defined by the atomic coordinates, to identify the feasible stable structures as local minima of the energy landscape, and to decide which one is preferred at a particular temperature and pressure

I. Siloi, V. Carnevali, B. Pokharel, M. Fornari, R. Di Felice, *Quantum Mach. Intell.* **3**, 3 (2021)
V. Carnevali, I. Siloi, R. Di Felice, M. Fornari, *Phys. Chem. Chem. Phys.* **22**, 27332 (2021)

Adiabatic quantum optimization

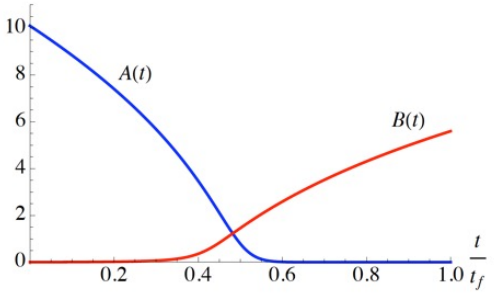
- Solve using AQO

Find the ground state of the Ising Hamiltonian

$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

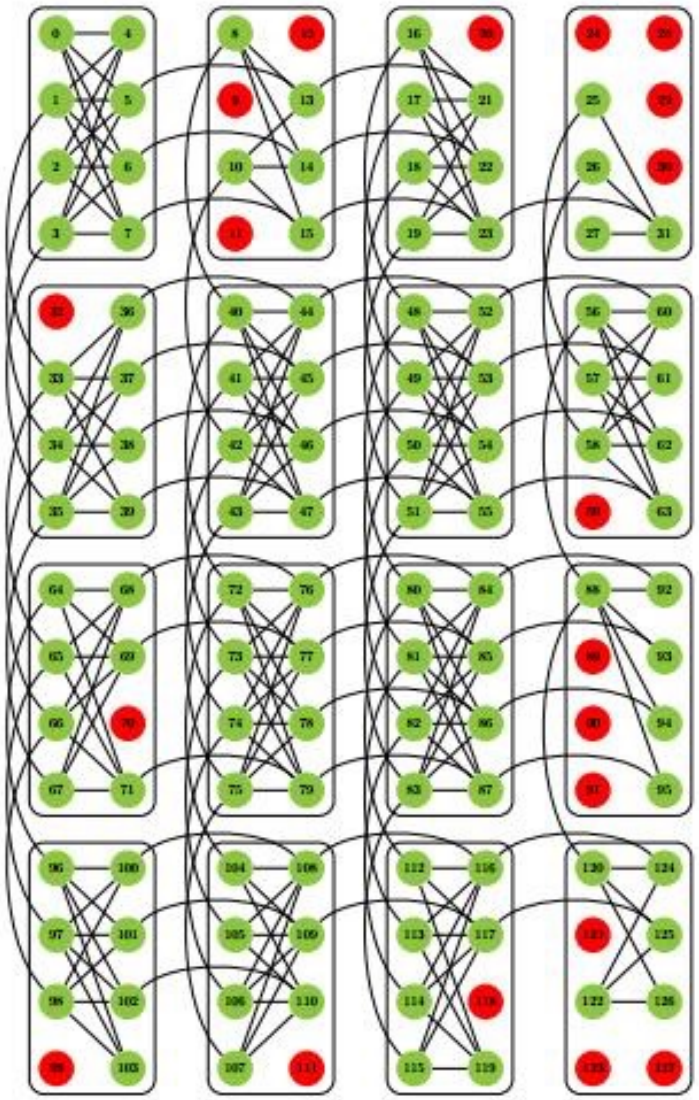
using adiabatic interpolation from the transverse field (Farhi et al., 2000)

$$H(t) = A(t) \sum_j \sigma_j^x + B(t) H_{\text{Ising}} \quad , \quad t \in [0, t_f]$$



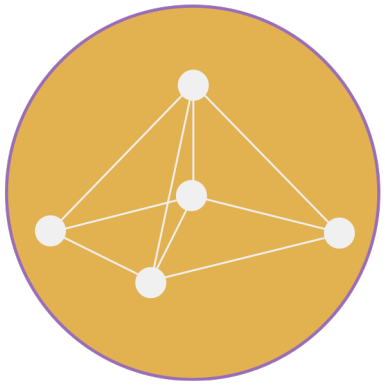
- Programming means finding the appropriate $\{h_i, J_{ij}\}$

Connectivity



Limitations on D-Wave

- **Graph completeness**
  - Minor embedding
  - D-Wave built-in function [J. Cai et al, ArXiv:1406.2741, 2014]
  - Truncation of data
- **Values of Ising parameters**
  - $-1 < h_i, J_{i,j} < 1$
  - Data normalization needed



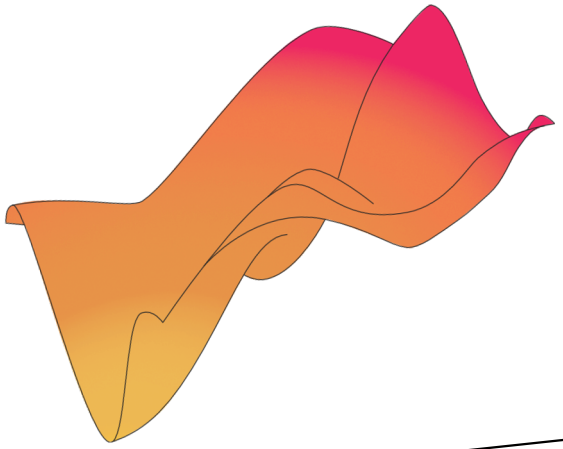
MELTING: AMORPHOUS SILICON

Competition between

short and long range order

Energy landscape exploration

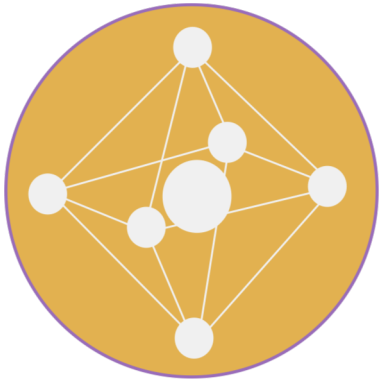
Combinatorial complexity

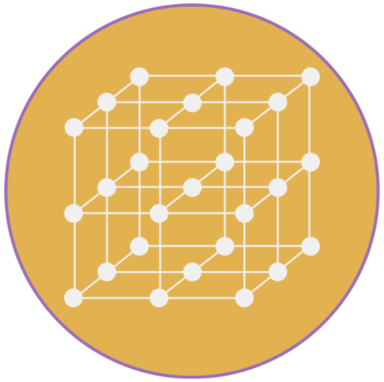


ORDER_DISORDER TRANSITIONS: $AB0_3$ PEROVSKITES

Competition between

order and disorder



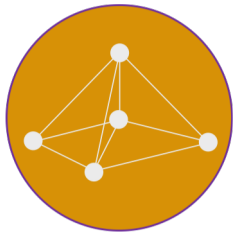
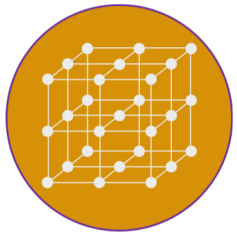


ENTROPY STABILIZATION HIGH ENTROPY ALLOYS

Competition between

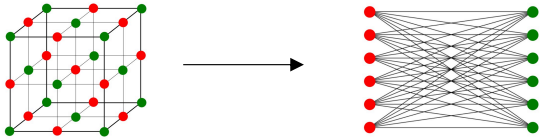
energy and entropy

D-Wave as a structural model generator


PROTOCOL

FROM CRYSTAL STRUCTURE TO NETWORK



atomic sites → nodes $\{v_i\}$

bonds → edges $\{e_i\}$

$G\ \{V, E\}$

QUBO DESIGN

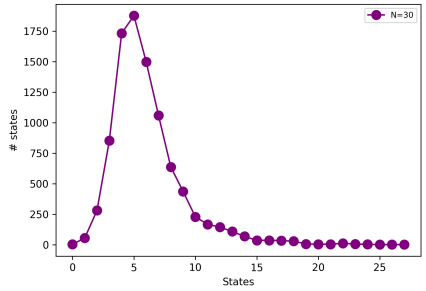
$$Q(x) = p_1 P_1(x) + p_2 P_2(x) + \cdots$$

$Q(x) = 0$ Ground state

$Q(x) \neq 0$ Excited states

EXCITED STATES have a PHYSICAL MEANING

STATISTICAL APPROACH



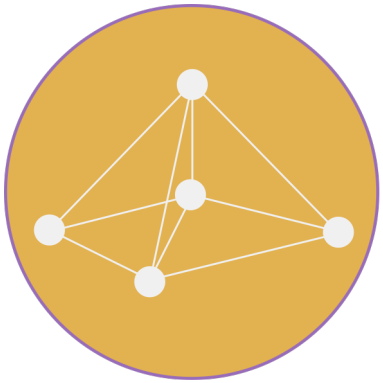
RUNNING the AMOUNT OF TIMES necessary to have the RIGHT STATISTICS

CLASSICAL SIMULATIONS

computational time limitation

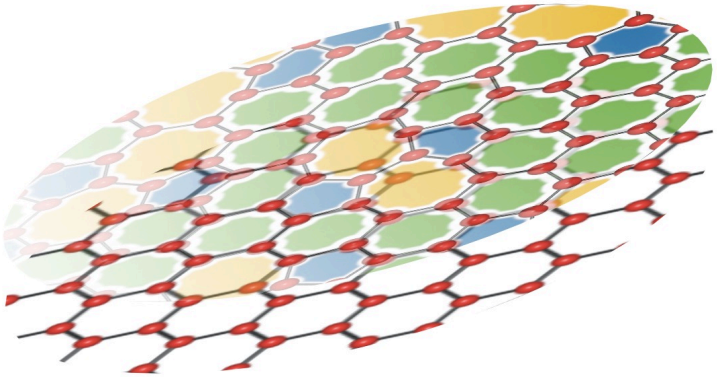
dependence on the initial conditions

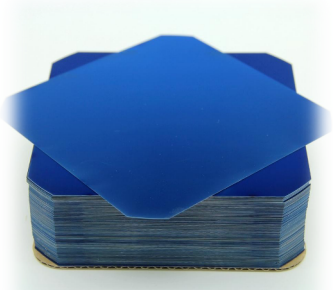
Amorphous Silicon



Competition between

short and long range order





Application to solar cells and

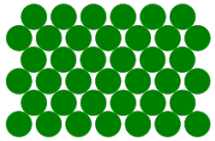
disordered systems

Generating structural models for

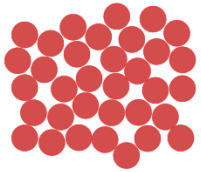
non-crystalline materials

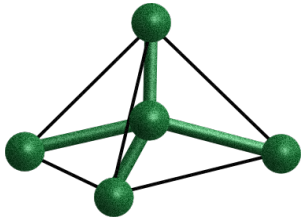
Amorphous Silicon

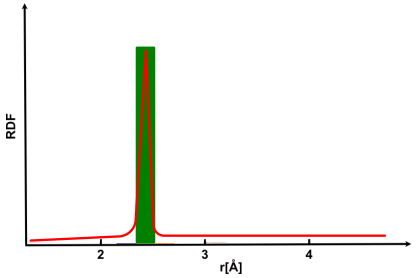
CRYSTALLINE



AMORPHOUS

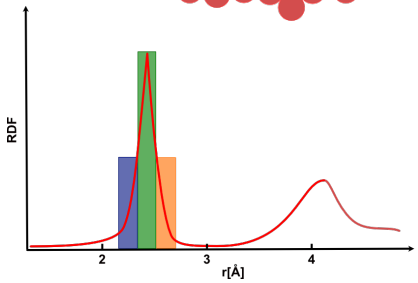


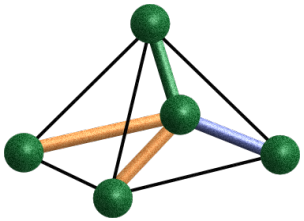




Radial Distribution Function

Bonds length distribution in the crystal





$$x = \{x_{i\alpha_n}\}$$

Silicon structural model as string of binaries: encoding #bonds and available bond lengths

GROUND STATE

$Q(x) = 0$

$$Q(x) = p\sum_i \left(1 - \sum_n x_{i\alpha_n}\right)^2 + \sum_{i,n} |\alpha_n - \alpha_c| x_{i\alpha_n}^2 + \sum_n \left(N_{\alpha_n} - \sum_i x_{i\alpha_n}\right)^2$$

Length of a certain bond is unique

How shrunk/ stretched the bonds are

How many bonds are not crystalline

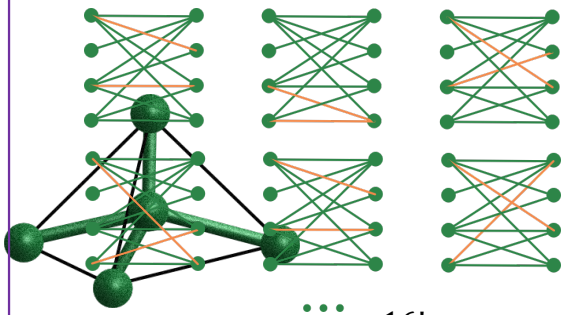
EXCITED STATES

$Q(x) \neq 0$

tuning *p* !

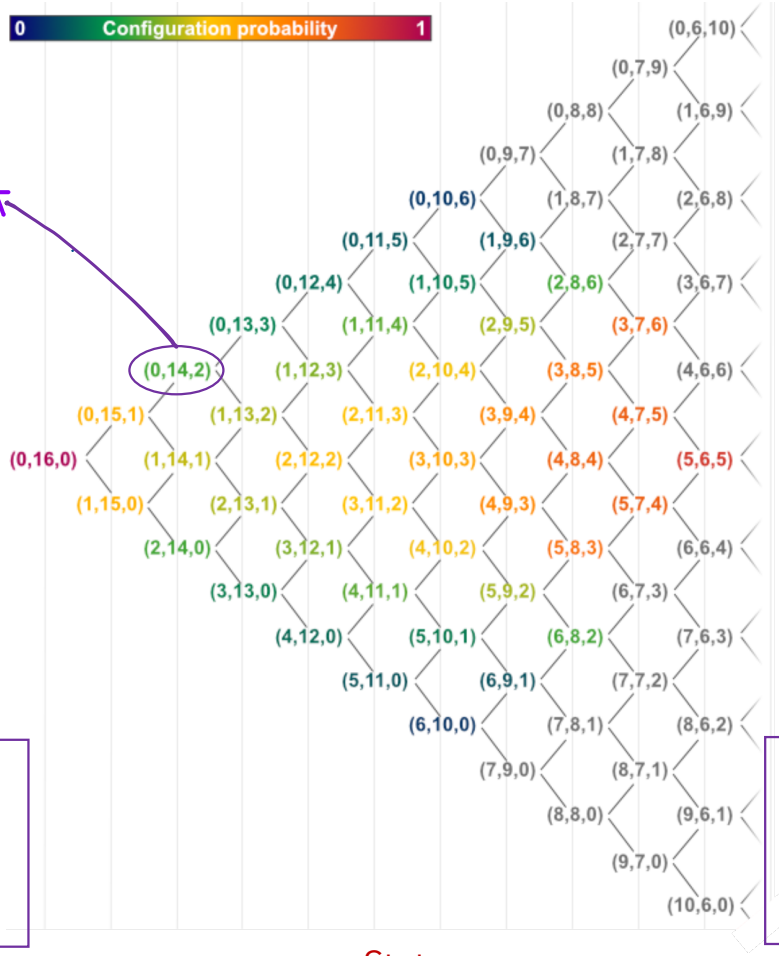
Structural models for Silicon

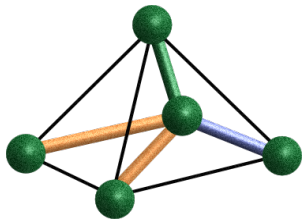
STRUCTURAL MODELS



$$\#structures = \frac{16!}{14!\,2!} = 120$$

CRYSTALLINE





AMORPHOUS

FILTERING EXCITATIONS

Binary strings that do not respect constraints are filtered out *a posteriori*

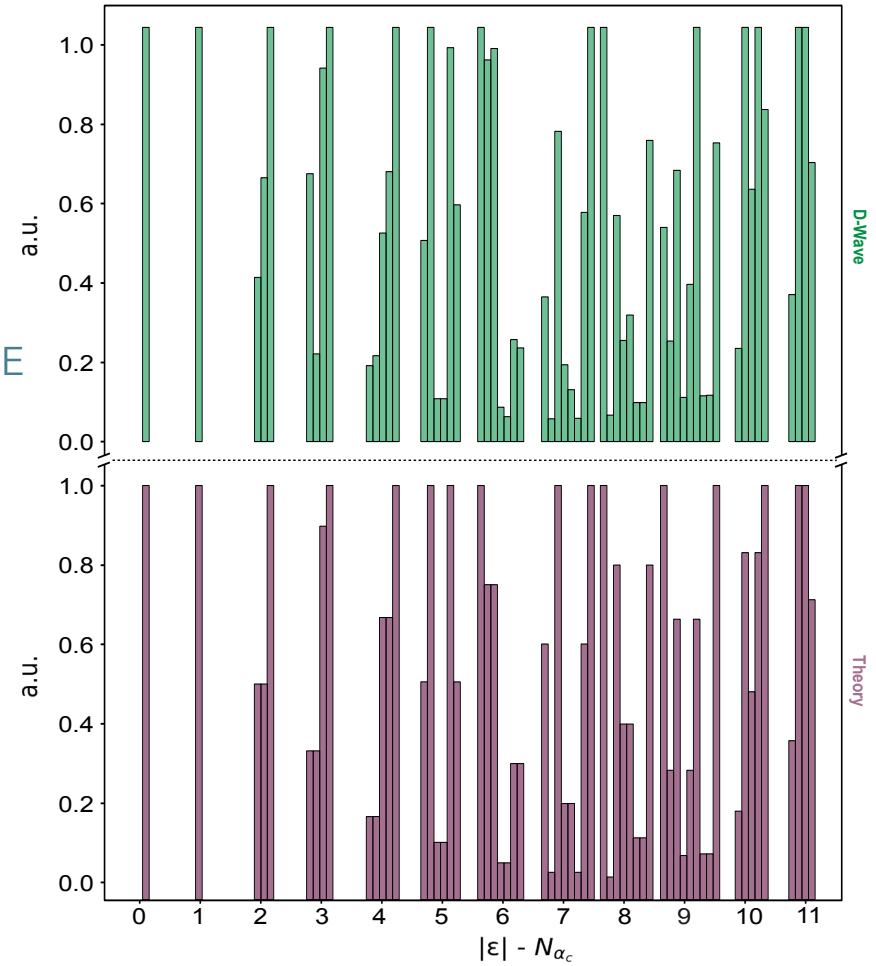
DETAILS

- Conventional cell with 8 atoms, 16 bonds
- 48 binaries, 408 couplings, 437 qubits

Structural models for Silicon

HOW MANY MODELS ARE FOUND BY DWAVE?

- distribution of models from DW close to theoretical one
- Increasing the statistics



Non-crystalline bonds

OBSERVATIONS

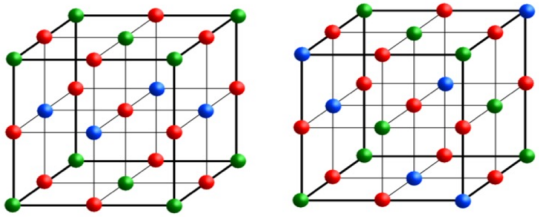
DW as a quantum generator of structural models

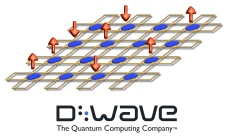
Better resolution with improving statistics

General approach extendable to more complex cases

Summary

Encoding stable and metastble states in the GROUND and EXCITED STATES OF A QUBO formulation





STATISTICS inherent in QUANTUM ANNEALING allows in principle the access to ALL STRUCTURAL MODELS