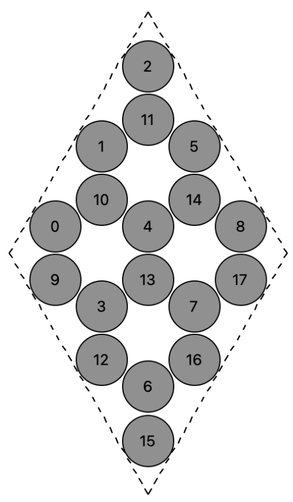
Quantum Annealing Applications for Quantum Chemistry

Goal	Method	Test model
Predict lowest energy configuration of solid solutions	Quantum annealing, D-Wave machines	Simulate vacancies in graphene

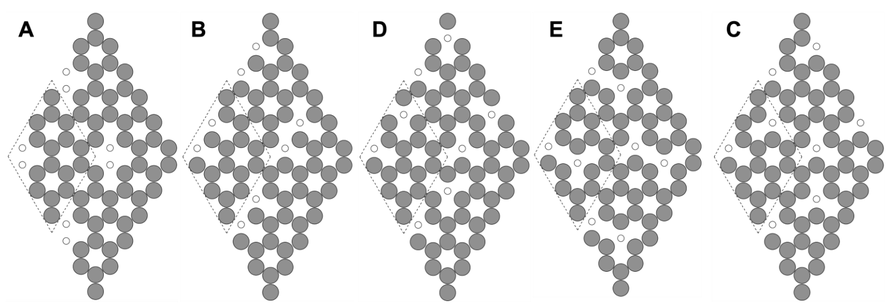
Binary Quadratic Model (QUBO)



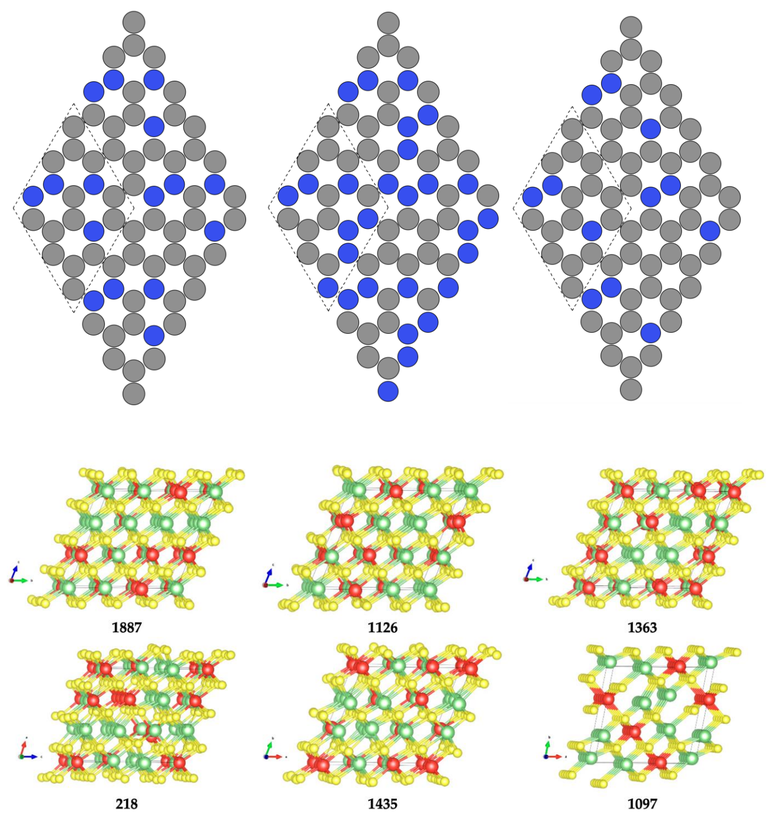
$$\alpha \underbrace{\sum_{i}^{N_{sites}} \sum_{j>i}^{N_{sites}} -A_{i,j}x_i x_j}_{\text{broken bonds objective}} + \beta \underbrace{\sum_{i}^{N_{atoms}} \sum_{j>i}^{N_{atoms}} -B_{i,j}x_i x_j}_{\text{coord objective}} +$$

$$+ \underbrace{\lambda \left(\sum_{i}^{N_{sites}} \left(1 - 2N_{atoms}\right) x_i + \sum_{i}^{N_{sites}} \sum_{j>i}^{N_{sites}} 2x_i x_j \right)}_{\text{constraint}}$$

$$\binom{N_{sites}}{N_{vac}} = \frac{N_{sites}!}{N_{vac}!(N_{sites} - N_{vac})!}$$



	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	% broken chains	Energy	% occurence
A	1	1	1	1	1	0	1	1	1	1	1	0	1	1	1	1	1	1	0.284900	-20.0	75.0
B	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	1	1	0.793651	-19.0	3.6
C	1	1	1	0	1	1	1	0	1	1	1	1	1	1	1	1	1	1	0.000000	-19.0	10.7
D	0	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	0.000000	-19.0	3.9
E	1	1	1	1	1	1	1	0	1	1	1	0	1	1	1	1	1	1	1.010101	-19.0	2.0



DFT calculated interaction energies

D-Wave Quantum annealing

Configurational analysis + Thermodynamic properties

SCAN ME!

QEVEC

D-wave demo

simulating
atomic vacancies
In graphene

Quantum Enhanced Verified Exascale Computing

ExCALIBUR
CROSS-CUTTING PROJECT

UKRI

Quantum Computing & Simulation Hub

ExCALIBUR 10