

Unstable crystal structure

Augmented lattice

Structure generation

Voronoi tessellation

Relaxation inside
Voronoi cell

Force constant

Monte Carlo
Markov chain

Vibrational
free energy

Ab initio calculations

P⁴ toolkit

ATAT toolkit

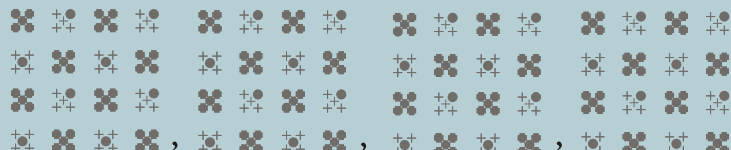
Configurations

(1)

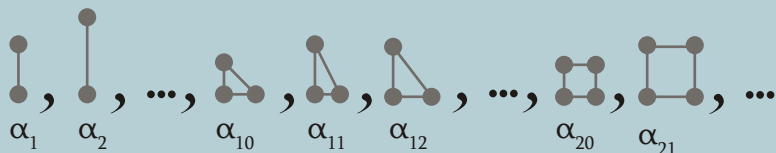
(2)

(3)

(4)



Clusters



$$F^{*(1)} = \sum_{\alpha} J_{\alpha} \sigma_{\alpha}^{(1)}$$

$$F^{*(2)} = \sum_{\alpha} J_{\alpha} \sigma_{\alpha}^{(2)}$$

$$F^{*(3)} = \sum_{\alpha} J_{\alpha} \sigma_{\alpha}^{(3)}$$

\vdots

J_{α}

$$F^* = \sum_{\alpha} J_{\alpha} \sigma_{\alpha}$$

Monte Carlo
Sampling