SI²: Automated Statistical Mechanics for the First-Principles Prediction of Finite Temperature Properties of Crystals

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CASM software package (a Clusters Approach to Statistical Mechanics)

Input
Crystal structure

Degrees of freedom
- Chemical
- Displacement
- Magnetic
- Molecular orientation

CASM-Hamiltonian
Algorithmic construction of effective Hamiltonians

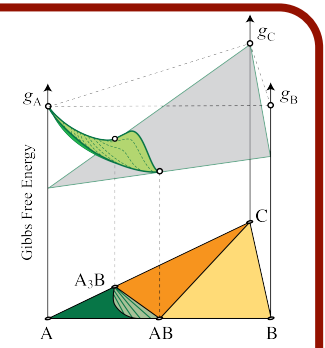
$$E\left(\vec{\sigma},\vec{u},\vec{s},\vec{q}\right) = V_o + \sum_{\alpha}\sum_{\vec{n}} V_{\alpha}^{\vec{n}} \cdot \Phi_{\alpha}^{\vec{n}}\left(\vec{\sigma},\vec{u},\vec{s},\vec{q}\right)$$

Cluster expansion

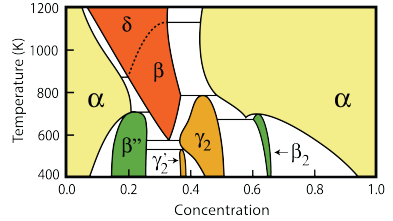
Symmetry adapted cluster basis functions

CASM-Monte Carlo
Equilibrium and kinetic Monte Carlo simulations

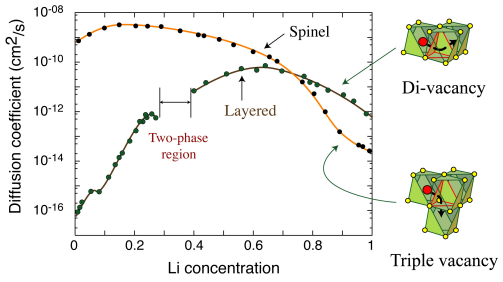
Free energies



Phase diagrams



Diffusion coefficients



CASM-Enumerate
Enumeration of symmetrically distinct excitations

First-principles Electronic structure code
(VASP, Quantum Espresso, FHI AIMS,…)

CASM-Learn
training of effective Hamiltonian expansion coefficients

scikit learn