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Articles

Article 1

Sampling Polymorphs of Ionic Solids using Random Superlattices

Article 2

Ab initio random structure search

Article 1

"Packing" Polymorphs

Solids with similar stoichiometry but different crystal structure/packing.

Polymorphs are found at the bottom of funnels

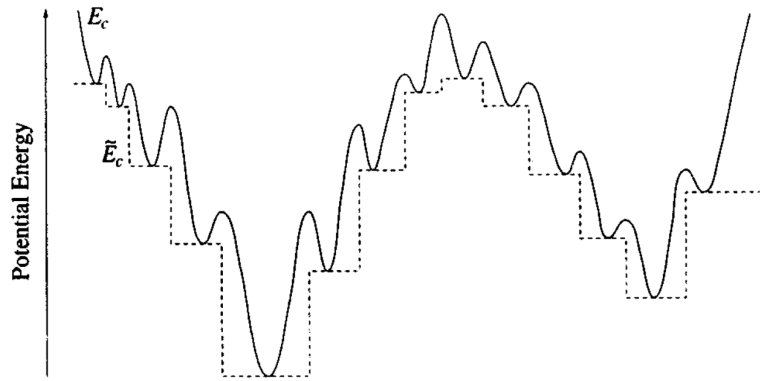


Figure: Two funnels containing multiple basins

Article 1

Factors influencing realizability of polymorphs

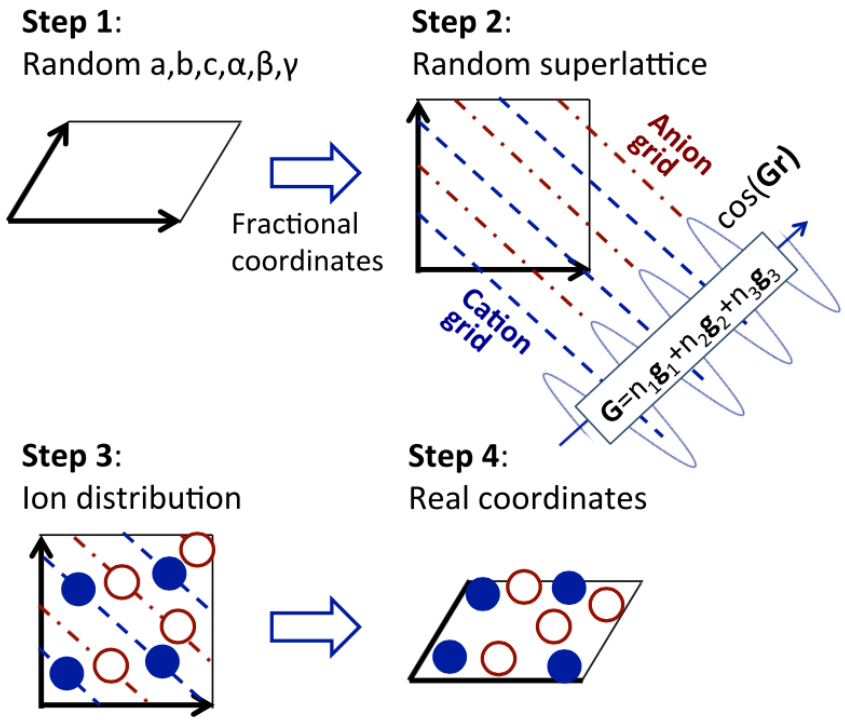
1. Energy above ground state
2. Energy barrier to escape minimum
3. Volume of configuration space occupied by the minimum of the polymorph.

This article focuses on assigning configuration space volumes.

The third factor might be a simplification as the volume of the whole funnel will probably contribute to the minimum basin of the funnel, as a result of annealing.

Article 1

Sampling using Random Superlatices



Article 2

Complexity of PES - motivational argument

1. Consider deviding a system of N atoms into M subsystems.
2. Assume that the M subsystems are large enough to have independent stable configurations.
3. Neglecting changes in the number of stable configurations arising from combining the M sub systems.

The total number of stable configurations $n_s(N)$ must then satisfy

$$n_s(N) = (n_s(N/M))^M$$

with solution

$$n_s(N) = \exp^{\alpha N}$$

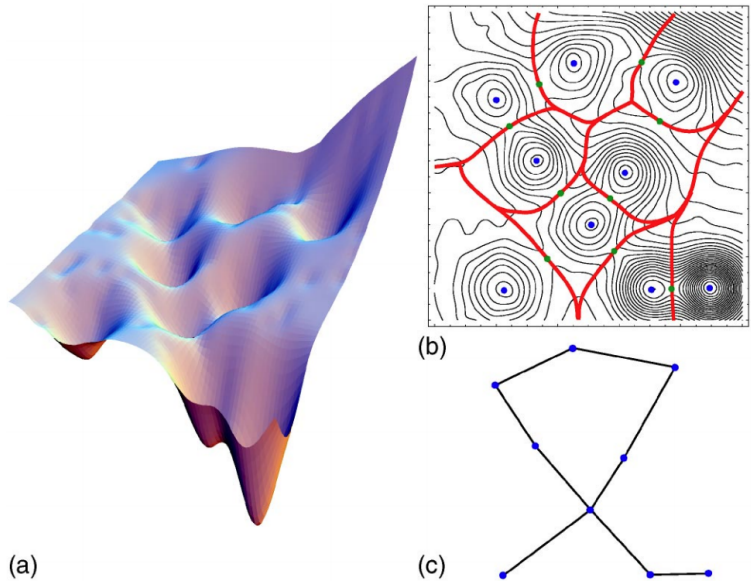
Article 2

General remarks on the PES

1. Almost no minima when atoms are close
2. The barrier to lower lying minima are smaller than those to higher lying minima
3. Low energy basins come in groups
4. Low energy basins occupy larger configuration space volumes

The distribution of number of transitions connecting a minima has a power law tail. The low

energy minima are highly connected.



t-SNE

- Nonlinear dimensionality reduction
- Maps points such that similar points remain close in the reduced space.
- Uses: Mapping to 2 or 3 dimensions, visualizing neural network representations.

Investigation of the PES

- DFT vs. DFTB+
- PES of molecules vs. solids