# Predicting Polymorphism in Partially Ionic Solids

## Scientific Achievement

We developed a theoretical approach to search for *new* and *realizable* metastable polymorphs in ionic systems.

## Significance and Impact

This approach will enable polymorphic materials to be incorporated in theory-guided materials searches (Materials by Design) so as to develop new functional materials.

## Research Details

**Structure Prediction:** Local DFT relaxations on a large set of random superlattices (RSLs) with quasi-random atom distribution on the RSL planes to promote realistic cation-anion coordination.

**Polymorph Realizability:** The occurrence frequency in RSL sampling is a measure for the basin-of-attraction size, i.e., the probability of "falling" into a given structure. All observed polymorphs of MgO, ZnO, and $SnO_2$ are shown to be the top-occurring structures, in agreement with experiment.

**Next Steps:** Application of this method (*Polymorph Sampler*) to to the design and discovery of *realizable* functional polymorphic materials.

V. Stevanovic, submitted (2015).

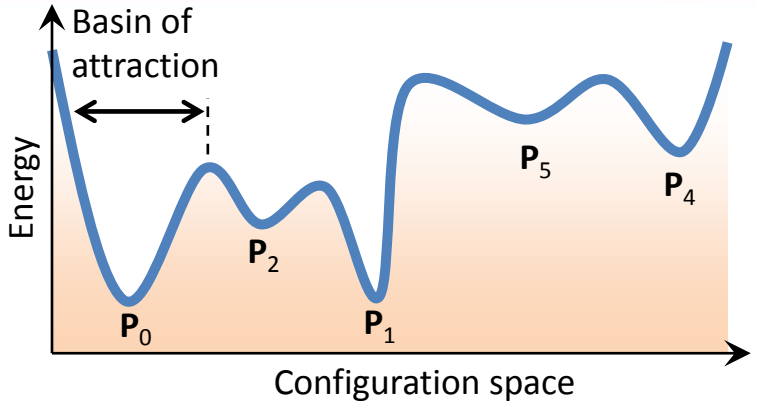


**Fig. 1.** Potential energy surface with polymorphs at the local minima, each having a basin of attraction.

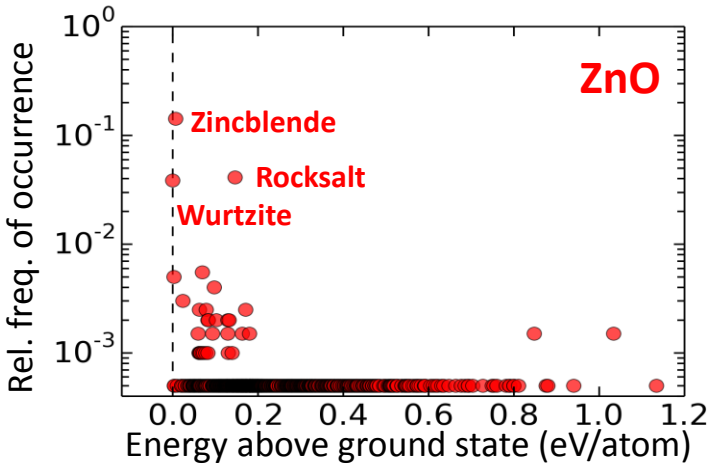


**Fig. 2.** The three realized ZnO polymorphs are the top-occurring structures in the RSL sampling.

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