Incorporating Metastable Polymorphs into Materials by Design

Scientific Objective

Create a high-throughput computational tool based on first-principles theory to predict the formation energy of polymorphs including new unknown structures.

Potential Significance and Impact

To date, the search space for Materials by Design (MdB) has been constrained to thermodynamic ground-state materials and already-known metastable materials. Yet, currently about two-thirds of new inorganic materials discovered each year are metastable. Hence, the inclusion of yet-to-be-discovered metastable materials into the MbB search space is critical.

Details

- Known polymorph materials (Fig. 1) provide a key basis set to test Polymorph Sampler, CNGMD's new tool to enable predictive discovery of new polymorphs.
- Polymorph Sampler will combine structure generation (from both random and prototype structures) with high-throughput total-energy calculations and data mining to identify all potentially synthesizable polymorphs.
- Looking forward, Polymorph Sampler v2 will use results from CNGMD's *Predictive Synthesis* thrust to add metrics addressing synthesizability and stability beyond just energy above the convex hull (ground state).

* Mn-O polymorph data from the Materials Project (DOE BES grant no EDCBEE)

Mn-O Polymorphs*

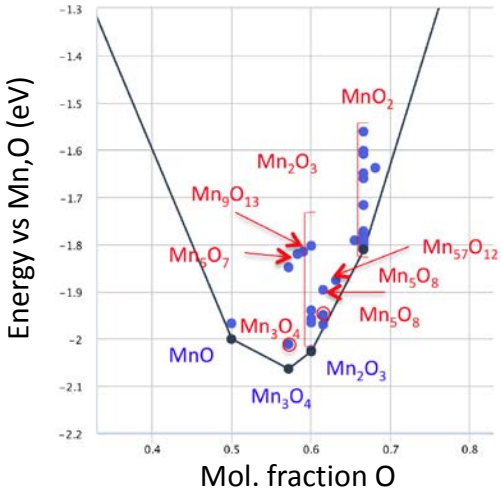

Fig. 1: Calculated formation energies of known and potential Mn-O polymorphs and stable convex-hull compounds (black dots).

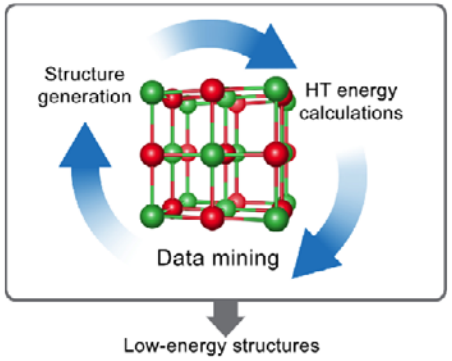

Fig. 2: Polymorph Sampler will add not-yet-discovered polymorphs to Materials by Design.

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