

# 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)

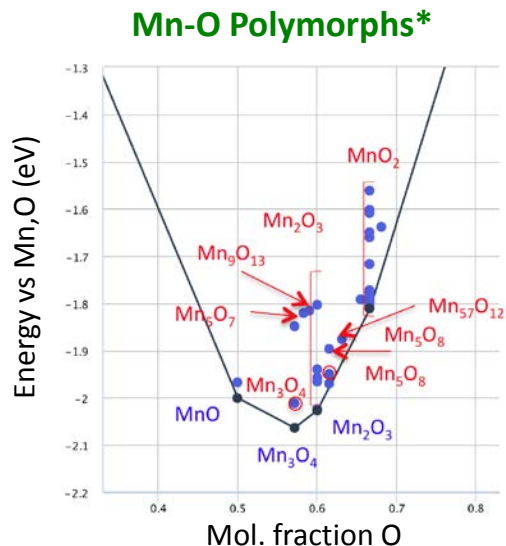


Fig. 1: Calculated formation energies of known and potential Mn-O polymorphs and stable convex-hull compounds (black dots).

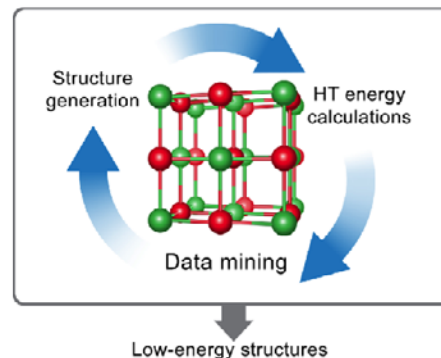


Fig. 2: Polymorph Sampler will add not-yet-discovered polymorphs to Materials by Design.