The Thermodynamic Scale of Inorganic Crystalline Metastability

Scientific Achievement

Revealed the thermodynamic landscape of inorganic crystalline metastability. Proposed principle of *Remnant Metastability*: "Observable metastable phases are remnants of thermodynamic conditions where they were once the lowest free-energy phase."

Significance and Impact

Metastable materials offer promising new design opportunities for high-performance materials. Accordingly, understanding their thermodynamics is key toward developing a predictive *ab initio* theory for guided materials synthesis.

Research Details

- Using the Materials Project as a materials informatics platform, 29,902 observed phases were data mined to reveal new insights into how chemistry and composition influence the accessibility of metastable polymorphic and phase-separating inorganic solids.
- Determined that many hypothetical low-energy metastable compounds may not be synthesizable, indicating a need for stringent synthesizability criteria in addition to the necessary condition of a low energy above the ground state.

W. Sun, S.T. Dacek, S.P. Ong, G. Hautier, A. Jain, W.D. Richards, A.C. Gamst, K.A. Persson, G. Ceder, *Science Advances* **2**, e1600225 (2016).

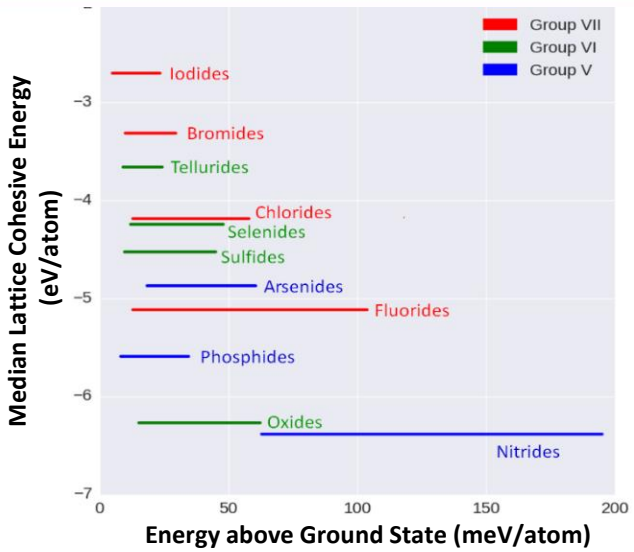

Fig. 1: ΔH above ground state as a function of chemistry. Within Groups, metastability scales with cohesive energy.

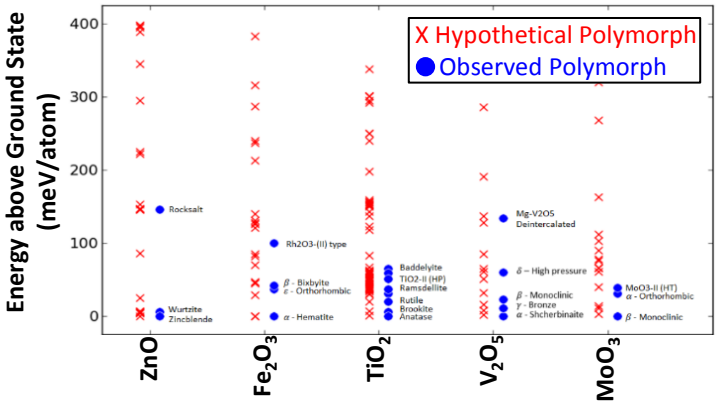

Fig. 2: *ΔH* above ground state for observed polymorphs (blue) and hypothetical, unobserved polymorphs (red).

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