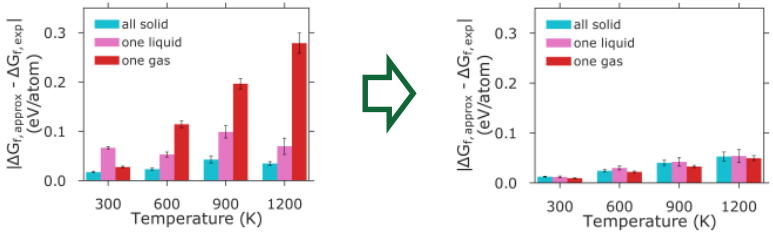
Physical Descriptor for the Gibbs Energy of Inorganic Crystalline Solids and Temperature-Dependent Materials Chemistry

Scientific Achievement: Developed a machine-learned descriptor enabling the chemically accurate high-throughput prediction of temperature-dependent thermodynamics (<40 meV/at MAE).

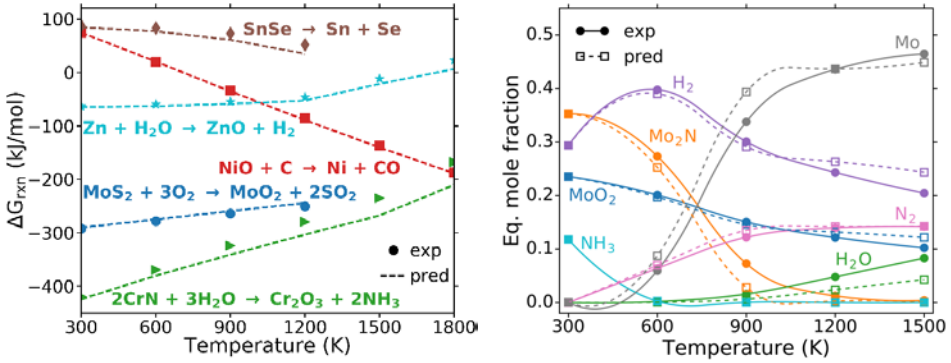


Significance and Impact: Provides the first comprehensive look at materials stability and synthesizability across the known inorganic crystalline compounds.

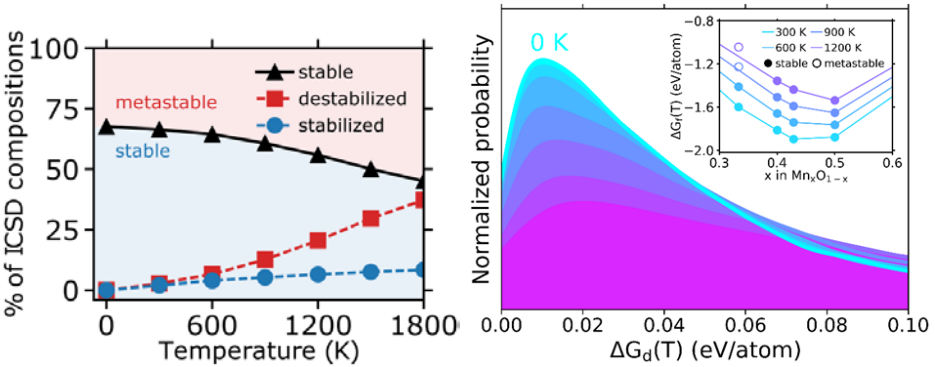
- Establishes the temperature-dependent scale of metastability.
- Identifies chemical design rules and compositions for realizing new, and likely synthesizable, highly metastable materials.

Research Details: Use the SISSO approach to identify an accurate, fast descriptor for *G(T)*. Apply this descriptor to generate and analyze **millions** of *T-x* **phase diagrams** (up to1,800 K) for more than **20,000 compounds** curated from the ICSD.

High-throughput prediction of $G_{rxn}(T)$ and reaction equilibria



Stability and metastability of inorganic compounds



C. Bartel, S. Millican, A. Deml, J. Rumptz, W. Tumas, A. Weimer, S. Lany, V. Stevanović, C. Musgrave, A. Holder, *Nature Communications* **9**, 4168 (2018).

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