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 to 1,800 K) for more than 20,000 compounds curated from the ICSD.

High-throughput prediction of $G_{\text{rxn}}(T)$ 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).