A Map of the Inorganic Ternary Metal Nitrides

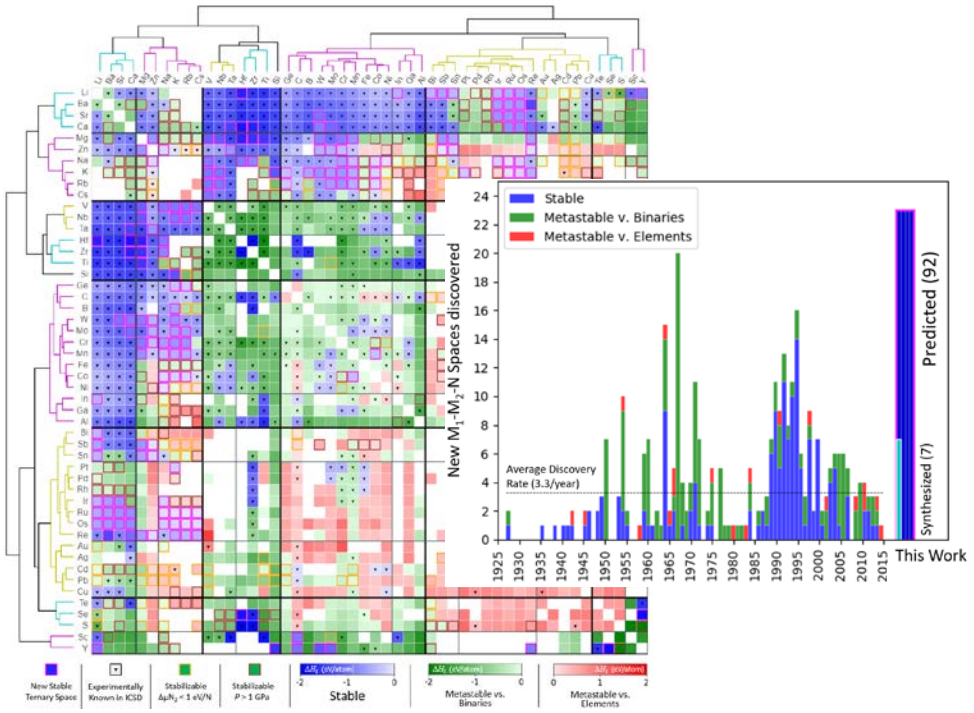
Scientific Achievement: We constructed the first comprehensive stability map of inorganic ternary metal nitrides to understand the chemical origins of stability and to predict new nitrides, along with the corresponding synthetic routes to realize them.

Significance and Impact: The map (to the right) clusters the ternary nitrides into chemical families with distinct stability and metastability, and it highlights hundreds of promising new ternary nitride spaces for experimental investigation.

Research Details

- > *200 new ternary nitrides* predicted to be stable, 100s more predicted to be synthesizable using reactive N or high-pressure routes. *Experimental realization: 7 attempted, 7 made (so far)*
- Data-driven analysis of solid-state bonding reveals the complex interplay between chemistry, composition, and electronic structure in governing large-scale stability trends in ternary nitride materials.
- Computational materials discovery (DFT, thermodynamic analysis) and materials informatics (data-mining, structure prediction, bonding and chemical analysis) tools were developed and used to map the entire class of ternary metal nitrides, guide the synthesis of new ternary metal nitrides, and identify large-scale chemical relationships.

A Map of Ternary Nitride Stability



Ternary $A_xB_yN_z$ Phases	Previously Known	Newly Predicted
Stable Ternary Phases	213	203
Metastable, ΔEHull < 70 meV/atom	92	417
Metastable, ΔEHull < 200 meV/atom	118	1213
Metastable: Stabilizable with ΔμN < +1 eV/N	3	92
Metastable: Stabilizable with Pressure ≥ 1 GPa	43	485

W. Sun, C. Bartel, E. Arca, S. Bauers, B. Matthews, B. Orvananos, B.R. Chen, M.F. Toney, L.T. Schelhas, W. Tumas, J. Tate, A. Zakutayev, S. Lany, A. Holder, G. Ceder, "A Map of the Inorganic Ternary Metal Nitrides," *Nature Materials* **18**, 732–739 (2019).

U.S. DEPARTMENT OF ENERGY | Office of Science | NREL | SLAC | BROOKHAVEN NATIONAL LABORATORY | HARVARD UNIVERSITY | OSU | University of Colorado Boulder | MINES | CNGMD Incorporating Metastability