# Materials Design Using Redox-Mediated Stabilization

#### **Scientific Achievement**

New, stable and metastable zinc molybdenum nitride (Zn-Mo-N) alloys with wurtzite-derived (wz) crystal structure have been theoretically predicted and experimentally synthesized. A broad range of properties—from insulating and transparent Zn<sub>3</sub>MoN<sub>4</sub> to conductive and absorptive ZnMoN<sub>2</sub>—is realized by tuning the composition.

# Significance and Impact

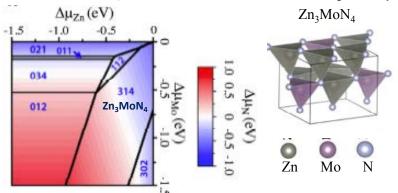
The successful synthesis of Zn-Mo-N materials demonstrates redox-mediated stabilization that is enabled by combining a multivalent cation (Mo<sup>6+</sup> or Mo<sup>4+</sup>) with a cation of intermediate electronegativity (Zn). This new design principle could lead to the discovery of many new ternary compounds.

#### **Research Details**

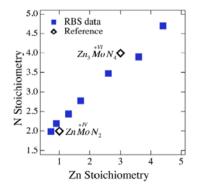
**Theory**: Data-mined ionic substitution for chemical space identification, followed by kinetically limited minimization for structure prediction.

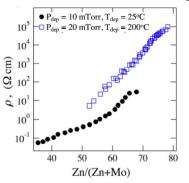
**Synthesis**: Composition gradient libraries on glass by co-sputtering of Mo and Zn metals in atomic N plasma.

### Theoretically Predicted Stable wz-Zn<sub>3</sub>MoN<sub>4</sub>



## Redox-Mediated Stabilization of wz-ZnMoN<sub>2</sub>





(Top): Theory predicts new stable  $Zn_3MoN_4$  and metastable  $ZnMoN_2$  in wurtzite-derived crystal structure. (Bottom): Experiments synthesize  $Zn_3MoN_4$ – $ZnMoN_2$  wurtzite alloys with composition-dependent electronic properties.

E. Arca, S. Lany, J.D. Perkins, C. Bartel, J. Mangum, W. Sun, A. Holder, G. Ceder, B. Gorman, G. Teeter, W. Tumas, and A. Zakutayev, *Journal of the American Chemical Society* **140**, 4293 (2018), DOI: 10.1021/jacs.7b12861













