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_3MoN_4 to conductive and absorptive $ZnMoN_2$—is realized by tuning the composition.

Significance and Impact

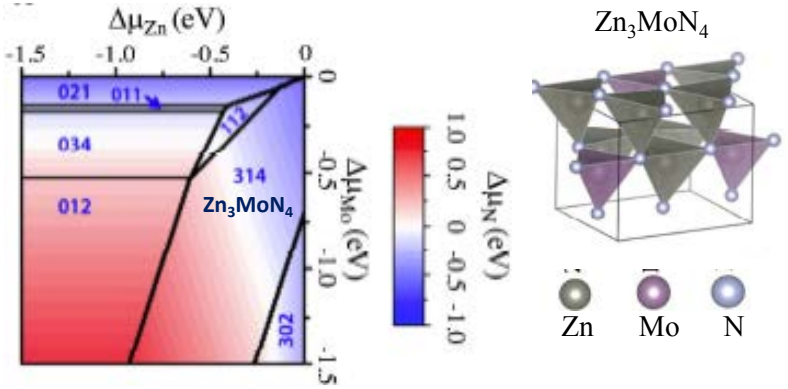
The successful synthesis of Zn-Mo-N materials demonstrates redox-mediated stabilization that is enabled by combining a multivalent cation (Mo^{6+} or Mo^{4+}) with a cation of intermediate electronegativity (Zn). This new design principle could lead to the discovery of many new ternary compounds.

Research Details

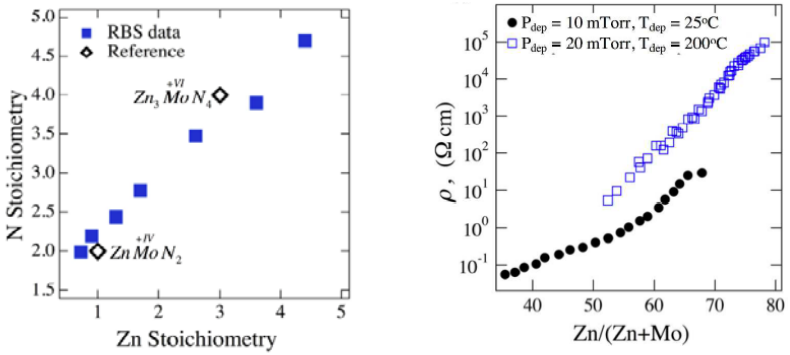
Theory: Data-mined ionic substitution for chemical space identification, followed by kinetically limited minimization for structure prediction.

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

Theoretically Predicted Stable wz-Zn_3MoN_4



Redox-Mediated Stabilization of wz-$ZnMoN_2$



(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

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