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$_3$MoN$_4$ 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.

(Top): Theory predicts new stable Zn$_3$MoN$_4$ and metastable ZnMoN$_2$ in wurtzite-derived crystal structure.