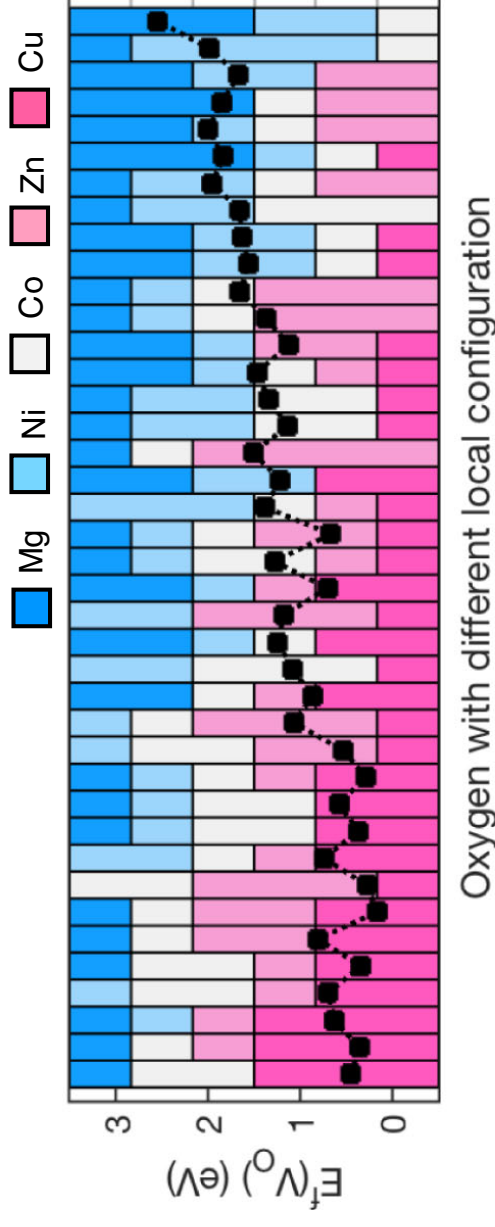


Entropic stabilization – the mixing of many different cations on one lattice site in a periodic crystal – provides a strategy to create new oxide materials and realize novel functional properties engineered through alloy composition. Achieving an atomistic understanding of these effects requires understanding how local compositional and structural disorder underlies structure-property relationships. MRSEC researchers have used high-throughput atomistic calculations to reveal how local configurational and structural disorder affects vacancy formation in (MgCoNiCuZn)O-based entropy-stabilized oxides, finding that cation-vacancy formation energies decrease with increasing tensile strain caused by variations in bond lengths caused by disorder. By applying charge-neutrality, researchers determined that the equilibrium concentrations of both oxygen and cation vacancies increase with increasing Cu mole fraction. Tuning the local chemistry and associated structural distortions by varying alloy composition enables controlled defect formation in multi-component alloys. As defects often control properties, this provides important insights towards applications of this emerging family of materials.



Variation in the defect formation energy with the local composition and structure of the high-entropy oxide, showing its importance.

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