Entropy for Emerging Functional Materials Design

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Abstract: Materials must rise to meet modern engineering challenges, including needs for greater efficiency, broader functionality, and improved stability. This application-driven demand necessitates new approaches to materials design leveraging broader structural and chemical selection spaces for improved properties and performance.

High-entropy oxides (HEOs) are an important emerging materials class for addressing these pressing challenges. Entropy — manifesting as sublattice disorder — confers structural stability, while elemental synergy supports tailorable property spaces unique from the chemical endmembers. The MRSEC IRG2 at Penn State leverages this concept of entropy as a design tool to research emergent functionality in novel crystalline oxides.

The IRG2 team employs experimental and computational tools to explore entropic contributions to phase stability and material properties across length dimensions, from bulk ceramics down to the nanoscale. We apply these tools across multiple crystalline classes, including rocksalt, perovskite, bixbyite, wolframite, and other structures. Through this approach, we can access large chemical selection spaces as well as diverse long-range and local symmetries, thereby enabling unique functional property responses. Notable property focus areas include transparent ion conductors, nonlinear dielectrics, and thermoelectrics, among others.

This approach exploits a much larger selection space than is available in conventional materials and highlights burgeoning opportunities for next-generation materials design.