Stability and Structural Distortion in Compositionally Complex Ceramics from First-Principles Calculations

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In the nuclear industry, many future technologies are limited by the availability of appropiate materials that can withstand the extreme environments created in next-generation fission or fusion reactors. Compositionally complex, or multi-principal component materials have several potential applications within the nuclear field due to potential improved properties over conventional materials. One example is "high-entropy" transition metal carbides, an emerging class of ultra-high temperature ceramics that have potential usage as structural materials in nuclear reactors or as protective coatings for aerospace applications, thanks to their apparent improved mechanical properties and oxidation resistance at extremely high temperatures. Another example is compositionally complex rare-earth oxides, which are being explored as hydrogen permeation barrier coatings in fusion applications, where it is believed that they show improved structural integrity under irradiation conditions.

Such compositionally complex materials are being explored initially by using simulations to navigate the vast combinatoric composition space. In many cases, high-throughout first-principles calculations are used to quickly assess promising compositions, while high-accuracy simulation is time consuming and computationally expensive. However, prediction of candidate materials is most effective when we have a mechanistic understanding of how the compositional complexity affects the desired properties, and so in-depth exploration is necessary.

This talk will explore high-accuracy density functional theory (DFT) simulations of "high-entopy" transition metal carbides and compositionally complex rare-earth oxides, giving examples of how atomistic simulation has been used to unveil key features that are the secret to the improved properties of these materials.