

# From High-Entropy Alloys to Warm-Dense Matter in a Single Framework: Thermodynamic Properties from KKR Multiple-Scattering Theory

Duane D. Johnson, Andrei Smirnov, Prashant Singh

*Iowa State University and Ames Laboratory; Markus Däne and Brian Wilson, Lawrence Livermore National Laboratory*

All-electron, KKR methods are presented that address electronic and thermodynamic properties of diverse materials systems from equilibrium, such as nascent short- and long-range order found in *high-entropy alloys* (having 5 or more components), to extremes, such as to *warm-dense matter* (exemplified on a NIF target material). KKR applications are discussed, including requirements in the theory and numerical methods to simulate and interpret properly complex alloys to materials over large pressure and temperature ranges. The all- electron KKR framework demonstrates its broad applicability and reliability.