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A computational study of high entropy alloys YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MICHAEL GAO, National Energy Technology Laboratory, MICHAEL WIDOM, Department of Physics, Carnegie Mellon University, JEFF HAWK, National Energy Technology Laboratory
— As a new class of advanced materials, high-entropy alloys (HEAs) exhibit a wide variety of excellent materials properties, including high strength, reasonable ductility with appreciable work-hardening, corrosion and oxidation resistance, wear resistance, and outstanding diffusion-barrier performance, especially at elevated and high temperatures. In this talk, we will explain our computational approach to the study of HEAs that employs the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. The KKR-CPA method uses Green's function technique within the framework of multiple scattering theory and is uniquely designed for the theoretical investigation of random alloys from the first principles. The application of the KKR-CPA method will be discussed as it pertains to the study of structural and mechanical properties of HEAs. In particular, computational results will be presented for $Al_xCoCrCuFeNi$ (x = 0, 0.3, 0.5, 0.8, 1.0, 1.3, 2.0, 2.8, and 3.0), and these results will be compared with experimental information from the literature.

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