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First-principles Calculations on the Stability of High Entropy Alloy[1] M. CLAUDIA TROPAREVSKY, Department of Materials Science and Engineering, the University of Tennessee, PAUL KENT, JAMES R. MORRIS, G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — High entropy alloys (HEAs) constitute a new class of materials comprised of four or more elements in equimolar or near equimolar ratio, which tend to form simple solid solutions, mainly FCC or BCC. Despite extensive attention due to their potential applications as structural materials little is known about why these compounds are stable with respect to phase separation. We study the structural and thermodynamic properties of HEAs composed of Cr, Pd, Mn, Fe, Co, and Ni using density functional theory. We investigate the minimum energy structures of several alloys as well as the competing intermetallic compounds in an effort to assess the stability of the HEAs with respect to phase separation. We find that the enthalpy of formation of the alloys is frequently insufficient to explain their stability and that the entropy of mixing can in some cases account for the stability of these compounds. However, for some five-component alloys this does not appear to be sufficient. In this presentation, we will discuss the degree to which the entropy of mixing can stabilize these alloys.

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