

Abstract Submitted
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Configurational entropy of solid solutions and high entropy alloys¹ MICHAEL WIDOM, Carnegie Mellon University — Multicomponent solid solutions such as high entropy alloys deviate from the ideal entropy of mixing owing to short-range chemical order among the constituent elements. The "mutual information" contained in correlation functions represents the entropy loss relative to ideal mixing. The entropy approximation of the cluster variation method is an example of this principle. We apply this method to estimate the configurational entropy of multicomponent body-centered cubic, partially ordered B2, and C15 Laves phase alloys using correlation functions obtained from first principles Monte Carlo/molecular dynamics simulations.

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