

First-Principles alloy thermodynamic properties based on cluster expansion

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This talk will review recent developments in the application of lattice-model effective Hamiltonians as a framework for first-principles modeling of alloy thermodynamic properties. Two examples will be described to highlighting applications in the design of multicomponent alloys, and the modeling of substitutional alloys with competing parent-lattice structures. Specifically, we will describe the use of first-principles calculations of the formation energies of ordered intermetallics in Al-TM-Zn (TM=Ti,Zr) alloys as a framework for aiding the design of new high-temperature Al alloys. We will also describe applications to the modeling of ordering and structural phase stability in Co-Pt alloys where first-principles calculations indicate a competition between surface and bulk ordering tendencies underlying the growth of thin films for magnetic-recording applications.