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First-principles calculations of free energies of solids

VIDVUDS OZOLINS, Dept. of Materials Science & Engineering, University of California, Los Angeles

Accurate *ab initio* calculations of the free energies of high-temperature solid phases present a long-standing problem in thermodynamics of materials. We show how density-functional theory molecular dynamics simulations in conjunction with thermodynamic integration over lattice strains can be used to obtain the free energy differences between the fcc, bcc, and hcp phases of metals. For the prototypical cases of Zr and W, we predict hcp/bcc and fcc/bcc energy and entropy differences that are in excellent agreement with the values derived from CALPHAD analysis of experimental data. The proposed methodology will find applications in first-principles calculations of thermodynamic properties and phase diagrams of metallic alloys, as well as in constructing accurate thermodynamic models of structural phase transformations.