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First-principles calculations of free energies of unstable phases: The case of fcc W[1] VIDVUDS OZOLINS, Department of Materials Science & Engineering, University of California, Los Angeles — Ab initio density-functional theory molecular dynamics simulations are used to solve the long-standing problem of calculating the free energies of harmonically unstable phases, such as fcc W. We find that fcc W is mechanically unstable with respect to long-wavelength shear at all temperatures considered (T>2500 K), while the short-wavelength phonon modes are anharmonically stabilized. The calculated fcc/bcc enthalpy and entropy differences at T=3500 K (308 meV and 0.74 kB per atom, respectively) agree well with the recent values derived from analysis of experimental data. The proposed method can be used in first-principles modeling of the thermodynamics of unstable phases and calculations of the thermodynamic driving forces for martensitic transformations in pure elements and alloys.

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