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First-principles calculations of lattice stabilities in Mo WESTON NIELSON, VIDVUDS OZOLINS, University of California, Los Angeles — The determination of accurate lattice stabilities is of great importance in producing phase diagrams of metallic alloys using the CALPHAD approach. Ab-initio molecular dynamics simulations in combination with thermodynamic integration are used to determine the lattice stabilities of fcc and bcc phases in Molybdenum at a range of temperatures. We employ the so-called fixed-cell-shape molecular dynamics approach, which involves the calculation of free energies over varying lattice strains. Our results also predict that at high temperatures fcc Mo is harmonically unstable.

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