# Metastable cubic and tetragonal phases of transition metals predicted by density-functional theory

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By means of density-functional calculations, we systematically investigated 24 transition metals for possible metastable phases in body-centered tetragonal structure (bct), including face-centered cubic (fcc) and body-centered cubic (bcc) geometries. A total of 36 structures not coinciding with equilibrium phases were found to minimize the total energy for the bct degrees of freedom. Among these, the fcc structures of Sc, Ti, Co, Y, Zr, Tc, Ru, Hf, Re, and Os, and bct Zr with $c/a = 0.82$ were found to be metastable according to their computed phonon spectra. Eight of these predicted phases are not known from the respective pressure-temperature phase diagrams. Possible ways to stabilize the predicted metastable phases are illustrated.

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