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First-principles study on the magnetic and structural properties of Fe-Co alloys¹ DANGXIN WU, PING LIU, QIMING ZHANG, The University of Texas at Arlington, RUQIAN WU, University of California, Irvine — $\text{Fe}_x\text{Co}_{1-x}$ alloys with different compositions are investigated using first-principles methods, FLAPW and PAW, based on density functional theory. The structural geometries of the alloys were optimized at a given composition by PAW method implemented in VASP. The initial structures were fcc and hcp for Co-rich systems, and bcc for Fe-rich systems. The formation energies were then calculated and the stability of the alloys was studied. For those systems with lower symmetries and favorable formation energies, the magnetic properties, such as the saturated magnetization and the magneto-crystalline anisotropy, were carefully studied using the FLAPW method.

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