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First-principles study of the electronic and magnetic properties of Fe-Co nanowires[1] DANGXIN WU, PING LIU, QIMING ZHANG, University of Texas at Arlington, RUQIAN WU, University of California, Irvine — Fe-Co nanowires provide a potential way to produce high-performance nanocomposite permanent magnets due to their high Curie temperature, large magnetization and appreciable anisotropy. In this talk we present our recent results of first-principles investigation of this matter. The calculations use both PAW method and FLAPW method, based on density functional theory. The structures of Fe-Co nanowires were optimized by PAW method and then the electronic structure and magnetic properties such as saturation magnetization and anisotropy energies are studied by FLAPW method. The effects of size and composition of the nanowires on the magnetic properties are also studied and compared with those of bulk Fe-Co materials.

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