An ab initio study of magnetism in nanocomposite Fe-Pd and Fe-Pt systems

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We perform a density functional theory study of ordered magnetic configurations in nanostructured Fe-Pd and Fe-Pt face-centered cubic (FCC) based intermetallics with low Fe content, namely FeX3, FeX7, FeX8 and FeX15 (X = Pd or Pt), that contain iron fibres in the platinum or palladium matrix.

The pseudopotential code VASP (Vienna Ab initio Simulation Package) is used to determine the equilibrium lattice parameters of the FCC-based structures and corresponding total energies.
Nonmagnetic, ferromagnetic and selected antiferromagnetic arrangements are considered and the configurations with the lowest energies are discussed in detail, including concentration dependence of both equilibrium volumes and magnetic moments.