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Self-consistent implementation of the vector disordered local moment method for magnetic alloys and its applications to magnetic thermodynamics KIRILL BELASHCHENKO, BHALCHANDRA PUJARI, University of Nebraska-Lincoln, PAUL LARSON, Colorado School of Mines, VLADIMIR ANTROPOV, Ames Laboratory, MARK VAN SCHILFGAARDE, King's College London — We describe an implementation of the coherent potential approximation within the LMTO formalism, which combines chemical and magnetic disorder treated within the vector disordered local moment model. It allows for arbitrary degree of magnetic order for Heisenberg spins specified by axially symmetric spin distribution functions. The atomic charges and potentials are determined self-consistently, and the transverse constraining fields are included as required by density functional theory. Total energies and spectral functions are available, and the spin distribution functions can be used as variational parameters to determine the magnetic state at the given temperature by minimizing the free energy. The performance of this method is illustrated using several examples. The predictions of the Curie temperatures by different approximations for several materials (such as Fe, Co, Gd, FePt, FePd, CoPt) are compared, including the effect of the constraining fields. We also discuss competing magnetic interactions in the $Fe_{1-x}Mn_xPt$ alloy, which is known from experiment to present five magnetic phases, including two noncollinear ones. We construct the magnetic phase diagram using the variational minimization of the free energy and obtain the correct sequence of phases.

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