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Self-consistent generalization of the disordered local moment (DLM) method for magnetically ordered systems at finite temperatures PAUL LARSON, KIRILL BELASHCHENKO, University of Nebraska — The disordered local moment (DLM) approach using the coherent potential approximation (CPA) has been integrated as a self-consistent addition to the tight binding linear muffin-tin orbital (LMTO) method. This Green's function routine coherently averages spin states in a method similar to that used for random alloys. In principle, the DLM method allows one to describe the electronic structure, magnetic thermodynamics, and transport properties of arbitrarily ordered magnetic states and their changes across magnetic phase transitions. However, existing implementations are limited to rotationally invariant paramagnetic states or do not treat the ordered states in a self-consistent fashion. The new version of DLM discussed here includes self-consistency of the angular distribution function and the angular-dependent site potentials in the ferromagnetic (or antiferromagnetic) state. As in the underlying LMTO code, arbitrary space groups and atomic bases are supported in the DLM approach. Preliminary results are given for transition metal systems as a function of temperature.

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