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Temperature dependence of the effective exchange and biquadratic coupling in ferromagnets: Calculation in the disordered local moment method PAUL LARSON, KIRILL BELASHCHENKO, University of Nebraska — We have implemented the disordered local moment (CPA-DLM) method within the tight-binding linear muffin-tin orbital (LMTO) basis. This implementation self-consistently determines the angular distribution function of the generalized Heisenberg model and the angular-dependent local potentials in the symmetry-broken state; the CPA procedure involves numerical integration over the polar angle of the spin. We present benchmark calculations for several materials including Fe, Co, FePd, FePt, and CoPt. We further extract the temperature dependence of the effective exchange and biquadratic coupling parameters from the angular dependence of the single-site grand potential. We find that the effective exchange parameter in Fe is almost temperature-independent, while the biquadratic interaction is entirely negligible at all temperatures. In FePd the effective exchange varies noticeably as a function of temperature, while the biquadratic coupling is somewhat more pronounced but still relatively small.

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