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Optimized Effective Potential Method for Non-Collinear Magnetism CLAUDIA AMBROSCH-DRAXL, SANGEETA SHARMA, JOHN K. DEWHURST, University Graz, NICOLE HELBIG, STEFAN KURTH, EBERHARD K. U. GROSS, Free University Berlin, SAM SHALLCROSS, Linköping University, LARS NORDSTRÖM, Uppsala University — A description of non-collinear magnetism in the framework of spin-density functional theory is presented for an exact exchange energy functional which depends explicitly on two-component spinor orbitals. The equations or the effective Kohn-Sham scalar potential and magnetic field are derived within the optimized effective potential framework. We have implemented this formalism within the full-potential linearized augmented planewave method, with an unconstrained magnetization density. Our calculations for Co and Fe show that the overestimation of moments seen in previous work was an artifact of the decoupled equations used. We further demonstrate, with the example of a magnetically frustrated Cr monolayer, how intra-atomic non-collinearity may be underestimated by local functionals.

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