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Beller Lectureship Talk: Exploring Exact Exchange for collinear and non-collinear magnetism[1]

CLAUDIA AMBROSCH-DRAXL, University of Leoben

In standard density functional theory, one usually describes exchange and correlation effects by approximations on the same footing, where typical examples are the local density approximation (LDA) and different flavours of the generalized gradient approximation (GGA). Only in recent years the exact exchange (EXX) or optimized effective potential (OEP) method has been investigated in more detail, where most of the work has been dedicated to semiconductors [1]. Here we explore the OEP approach for magnetic materials. We provide a general description of the method which comprises the case of non-collinear magnetism. The equations for the effective Kohn-Sham scalar potential and magnetic field are derived within this framework, where the exact exchange energy functional explicitly depends on two-component spinor orbitals. The example of a magnetically frustrated Cr monolayer shows [2] that the resulting magnetization density exhibits much more non-collinear structure compared to LDA. The finding that a time-dependent generalization of the non-collinear OEP method can be a promising approach for an *ab-initio* description of spin dynamics provides an interesting outlook for future work. In the present study, a series of materials is investigated in view of the reliability of the OEP method in terms of their magnetic properties.

[1] M. Städele, M. Moukara, J. A. Majewski, P. Vogl, and A. Görling, Phys. Rev. B 59, 10031 (1999).

[2] S. Sharma, J. K. Dewhurst, C. Ambrosch-Draxl, N. Helbig, S. Kurth, S. Shallcross and L. Nordström, and E. K. U. Gross, Phys. Rev. Lett. 98, 196405 (2007).

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