MAR11-2010-002982

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Orbital-dependent functionals in FLAPW: hybrid functionals and optimized effective potentials[1]

STEFAN BLÜGEL, Institut fuer Festkoerperforschung and Institute for Advanced Simulation, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany

Orbital-dependent functionals are a new class of exchange-correlation (xc) functionals for density-functional theory. Hybrid functionals combine a local or semi-local xc functional with a nonlocal orbital-dependent exchange functional and improve the band gaps of semiconductors and insulators as well as the description of localized states. As an alternative to nonlocal hybrid potentials, one can also construct local optimized effective potentials (OEP) from the exact exchange (EXX) functional. So far, most implementations for periodic systems use a pseudopotential plane-wave approach. We present an efficient all-electron, full-potential implementation of the PBE0 [1] and HSE [2] hybrid functionals as well as the OEP-EXX functional [3] within the FLAPW method (`Fleur` code: www.flapw.de). Results for prototype semiconductors and insulators are in very good agreement with other implementations. We will demonstrate the improvement over conventional local or semilocal functionals for oxide materials and focus in particular on systems where standard functionals yield qualitatively wrong results. In particular, we will discuss the geometric and magnetic structures of EuO and GdN. Additionally, we will address the possibility of using the hybrid-functional ground state as starting point for a *GW* quasiparticle correction [4] and show results for complex perovskite systems.

[1] M. Betzinger, C. Friedrich, and S. Blügel, Phys. Rev. B 81, 195117 (2010).
[2] M. Schlipf, M. Betzinger, C. Friedrich, M. Lezaic, and S. Blügel, inpreparation.
[3] M. Betzinger, C. Friedrich, S. Blügel, and A. Görling, to be published in Phys. Rev. B.
[4] C. Friedrich, S. Blügel, and A. Schindlmayr, Phys. Rev. B 81, 125102 (2010).

[1]Financial support from the DFG through the Priority Program 1145 and the Helmholtz association through the Young Investigators Group Program, contract VH-NG-409, is gratefully acknowledged.