Optimized-effective-potential method within the all-electron FLAPW approach

A talk by Markus Betzinger

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The optimized-effective-potential (OEP) method is a special technique to construct local effective Kohn-Sham (KS) potentials from general orbital-dependent energy functionals. We focus in this talk on the exact exchange (EXX) functional. The corresponding local potential results from the solution of the OEP integral equation, in which the KS density response enters.
We solve this integral equation within the all-electron full-potential linearized augmented-plane-wave (FLAPW) method by representing the local potential in terms of a mixed product basis. In this way, the integral equation turns into an algebraic equation [1], which can be solved for the local potential by standard numerical algebraic tools. We demonstrate that the mixed product and LAPW basis must be properly balanced to obtain smooth and converged EXX potentials without spurious oscillations. This balancing scheme can be traced back to the convergence behavior of the response function and requires uneconomically large LAPW basis sets.
As a solution we propose an incomplete-basis-set correction (IBC) for the response function [2]. The IBC utilizes the potential dependence of the LAPW basis functions and explicitly calculates the response of the basis with respect to a change in the potential by solving radial Sternheimer equations. The IBC contribution to the response function lies in general outside the Hilbert space spanned by the original basis set and thus captures response contributions that could not be determined from the standard sum-over-states expression of Rayleigh-Schrödinger perturbation theory. We show that the IBC considerably accelerates the convergence of the density response function in terms of the LAPW basis-set size and the number of unoccupied states. The IBC is crucial to obtain physical EXX potentials with the conventional minimal LAPW basis. Finally, we show EXX-OEP results for the 3d transition-metal oxides. The EXX functional consistently opens the KS band gap and most notably antiferromagnetic FeO and CoO are predicted to be insulating. As an outlook, a generalization of the IBC to frequency-dependent perturbations is discussed extending its application range to the RPA correlation energy functional. Work was done in collaboration with Christoph Friedrich and Stefan Blügel.

[1] M. Betzinger at al., Phys. Rev. B 83, 045105 (2011)
[2] M. Betzinger et al., Phys. Rev. B 85, 245124 (2012) , ibid. 88, 075130 (2013)