Implementation of the exact-exchange Kohn-Sham functional within the all-electron FLAPW method

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Abstract

The success of density-functional theory (DFT) relies on the availability of accurate approximations for the exchange-correlation (xc) functional. Standard xc functionals, such as the local-density and the generalized-gradient approximation, suffer from several shortcomings: an unphysical electronic self-interaction, no discontinuity of the xc potential at integral particle numbers, among synergistic behavior etc. Orbital-dependent functionals are a promising new generation of xc functionals. The simplest variant consistent with the Kohn-Sham theory requiring a local xc potential is the exchange functional (DHF) functional. It does not exhibit the above mentioned deficiencies. We implemented the EXX functional within the full-potential augmented-plane-wave (FLAPW) method as realized in the FLEUR code (www.fleur.de) using a specifically designed auxiliary basis set for the optimized effective potential (OEP) equation. We demonstrate that the auxiliary and FLAPW basis must be properly balanced to avoid spurious results in the exact exchange potential and show results for prototype semiconductors and insulators.

Orbital-dependent functionals

Orbital-dependent xc functionals of DFT are indirect functionals of the density, since the KS orbitals ψn,l are functionals of the effective KS potential Veff. Let us assume the density ρe is specified. In order to calculate the local xc potential for such a function the chain rule for functional derivatives must be applied:

\[ V_{xc}(\rho_e) = \sum_{n,l} \int d^3r \left( \frac{\partial^2 \delta \phi_n}{\partial \rho_e \partial \rho_e} \right)_{\Phi_n} \cdot \left( \frac{\partial \delta \phi_n}{\partial \rho_e} \right)_{\Phi_n} \]

where the density is specified, since the KS orbitals are functionals of the effective KS potential. We find that the auxiliary and FLAPW basis must be properly balanced to avoid spurious results in the exact exchange potential and show results for prototype semiconductors and insulators.

Results

We demonstrate for the case of diamond that a smooth and physical local xc potential exists. Results are provided for the silicon surface and for the FeB compound.

Conclusions

We have presented an implementation of the exact-exchange Kohn-Sham functional within the all-electron FLAPW method based on the mixed product basis. We have shown for the case of diamond that the local xc potential is spatially strongly correlated, which makes a full-potential treatment even more important than in conventional LDA or GGA calculations.

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