DFT and beyond using a multiple scattering approach

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The versatility of the multiple scattering KKR-Green's function (KKR-GF) method as a powerful tool for the determination of the electronic structure of solids is illustrated with two developments.

We present the formalism and implementation of a relativistic optimized effective potential method in the framework of exact exchange (EXX) within spin-DFT. All ingredients of the integral equation are expressed in terms of the KKR-GF, thereby avoiding a basis set formulation. The real-space static Kohn-Sham response function as well as the inhomogeneity of the integral equation are expressed in terms of the GF. In the all-electron formulation, core, valence and their respective cross terms are treated explicitly. By imposing appropriate boundary conditions the associated core part of the code can be used to calculate free (open-shell) atoms. [1,2] A formulation of the RPA within the scheme is sketched. We further give examples of the application of the method to solids using EXX. [3]

In the second part we present the formalism and an implementation of total energy calculations in the local density plus dynamical mean field theory (LDA+DMFT) method within KKR-GF. Applications of the scheme to fcc-Nickel and γ-Manganese are shown. [4,5]

Literature:

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