Materials Science and Technology Division

"Relativistic Optimized Effective Potential (OEP) Method for Solids"

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4515/HTML, Room 265

Abstract

We present the first implementation of a spin-polarized relativistic optimized effective potential method (ROEP) for solids in the framework of spin-density functional theory. We have reformulated the ROEP in terms of Green's functions and sketch our subsequent implementation within the framework of the KKR multiple-scattering theory for solids. This method is an all electron, basis set free approach. All quantities are expanded in a fully relativistic spin-angular representation; spin-orbit coupling is treated nonperturbatively. Core-core interactions are determined along the lines of the method presented in Ref. [1,2], core-valence (band states) and valence-valence interactions are expressed in terms of the relativistic multiple-scattering representation. We used exact exchange (EXX) as a first step towards a complete exchange correlation functional. Results for alkali and transition metals are discussed [3].

References

[1] D. Ködderitzsch, H. Ebert, E. Engel, Phys. Rev. B77, 045101 (2008)
[2] E. Engel, D. Ködderitzsch, H. Ebert, PRB 78, 235123 (2008)
[3] D. Ködderitzsch, H. Ebert, H. Akai, E. Engel, J. Phys: Condens. Matter, 21, 064208 (2008)

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