LINEAR RESPONSE AT THE 4-COMPONENT RELATIVISTIC DENSITY FUNCTIONAL LEVEL: THEORY AND APPLICATIONS

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Density functional theory (DFT) has become an efficient and widely used tool of modern quantum chemistry. It is therefore only natural to extend this approach to the relativistic domain, where the computational cost is generally higher. We have implemented DFT in the relativistic molecular package DIRAC[1], following a pragmatic approach based on the use of non-relativistic functionals (LDA,BLYP, B3LYP).

In this paper we report the implementation of DFT in the response module of the DIRAC code. Due to the general structure of this module and the availability of property integrals in the HERMIT code, this effort allows the calculation of a wide range of linear response functions, including the frequency-dependent dipole polarizability and NMR-parameters.

References

[1] Dirac, a relativistic ab initio electronic structure program, Release 3.2 (2000), written by T. Saue, V. Bakken, T. Enevoldsen, T. Helgaker, H. J. Aa.Jensen, J. K. Laerdahl, K. Ruud, J. Thyssen, and L. Visscher (http://dirac.chem.sdu.dk)