The Douglas-Kroll-Hess Approach to the Dirac-Kohn-Sham Problem. Methodological Aspects and Applications

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The Douglas-Kroll-Hess approach to relativistic density functional theory as implemented in the density functional software ParaGauss is reviewed. We will discuss methodological aspects of the scalar relativistic [1] and the spin-orbit variants including a treatment of open-shell systems. Spin-orbit effects will be exemplified for small molecules of heavy elements. We will present examples of all-electron applications to molecules, clusters, and adsorption systems where relativistic effects are important.

[1] N. Rösch, S. Krüger, M. Mayer, V.A. Nasluzov,
"The Douglas-Kroll-Hess Approach to Relativistic Density Functional Theory: Methodological Aspects and Applications to Metal Complexes and Clusters",
in:
Recent Developments and Applications of Modern Density Functional Theory,
J. M. Seminario (Ed.),
Elsevier, Amsterdam, 1996, p. 497-566.