Current status of the Relativistic Effective Core Potential method

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The relativistic pseudopotential or relativistic effective core potential (RECP) method with the pseudoorbitals (pseudospinors) smoothed in atomic cores is the most economical and popular approach exploited in calculations of molecules containing heavy atoms [1]. The smoothing allows one to reduce the number of primitive Gaussian basis functions required for appropriate description of valence spinors in subsequent molecular calculations and also to exclude the small components of the four-component Dirac spinors from the RECP calculations, with relativistic effects being taken into account by *j*-dependent effective potentials. In a series of papers (see [2] and references therein), we have introduced and developed the generalized RECP (GRECP) technique. In contrast to other RECP methods, GRECP employs the idea of separating the space around a heavy atom into three regions: inner core, outer core and valence, which are treated in the framework of different approximations. It allows one to attain practically any desired accuracy, while requiring moderate computational efforts since the overall accuracy is limited in practice by possibilities of correlation methods. Recently, new GRECP versions [3,4] were developed which can effectively account for the contributions from Breit interactions and correlations with the core electrons (excluded from the GRECP calculations). In the report, performance of the new GRECPs together with other well-known RECP versions is discussed and their accuracy is analyzed in atomic calculations as compared to the all-electron Hartree-Fock-Dirac-Breit values.

This work was supported by the RFBR grant 06-03-33060, A.P. is also supported by the Russian Science Support Foundation.

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