RELATIVISTIC COMBINED PSEUDOPOTENTIAL−RESTORATION METHOD FOR STUDYING MULTITUDE OF PROPERTIES IN HEAVY-ATOM SYSTEMS[a]

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The relativistic pseudopotential (RPP) calculations of valence (spectroscopic, chemical etc.) properties of molecules are very efficient because the modern two-component RPP methods allows one to treat very accurately the correlation and relativistic effects for the valence electrons of a molecule and to reduce dramatically the computational cost. The valence molecular spinors are usually smoothed in atomic cores and, as a result, direct calculation of electronic densities near heavy nuclei within such approach directly is impossible. Precise calculations of such properties, as hyperfine constants and other magnetic properties, parity nonconservation effects, which are described by the operators heavily concentrated in atomic cores, usually require very accurate accounting for both relativistic and correlation effects. Electronic structure should be well evaluated in both valence and atomic core regions. However, precise all-electron four-component treatment of molecules with heavy elements is yet rather consuming. In the report, an alternative approach based on the RPP method and one-center core-restoration technique [1] developed by the authors for such studies is discussed. Its efficiency is illustrated in benchmark to-date calculations of magnetic−dipole and electric quadrupole hyperfine−structure constants, as well as the space parity (P) and time-reversal symmetry (T) nonconservation effects in polar heavy-atom molecules, including HfF^+, PtH^+, ThO and WC, which are studied now as promising candidates for the experimental search of the electron electric dipole moment (eEDM).

[1] A.V.Titov, N.S.Mosyagin, A.N.Petrov, T.A.Isaev, D.DeMille, Progr. Theor. Chem. Phys., **15B**, 253 (2006).

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