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Relativistic Pseudopotential Followed by Restoration Method for Studying Heavy-Atom Systems[1] ALEXANDER PETROV, B.P.Konstantinov Petersburg Nuclear Physics Institute; Department of Physics, St. Petersburg State University, LEONID SKRIPNIKOV, NIKOLAY MOSYAGIN, ANATOLY TITOV, B.P.Konstantinov Petersburg Nuclear Physics Institute — Precise all-electron four-component treatment of molecules with heavy elements is yet rather consuming. In turn, the relativistic pseudopotential (RPP) method is the most straightforward way now to study efficiently "valence" (optic, electric, chemical etc.) properties of rather complicated systems. However, the valence molecular spinors are usually smoothed in atomic cores. Therefore, direct calculation of electronic densities near heavy nuclei within the RPP approach is impossible. In the report, an approach based on the RPP method and one-center core-restoration technique [1] developed by the authors for such studies is discussed. It 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^+, WC, PbF^+, PbO, YbF, ThO and some other candidates which are studied now as promising molecules 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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