Precise study of heavy-atom compound electronic structure to extract fundamental properties of electron and nuclei

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Search for the effects of violation of time-reversal and spatial parity symmetries of fundamental interactions is of key importance to test extensions of the standard model. The interactions can lead to nonzero value of permanent electric dipole moment of the electron (eEDM), nuclear magnetic quadrupole moment (MQM), nuclear Schiff moment (NSM), etc. Heavy-atom compounds are very promising systems to search for these fundamental characteristics. However, the interpretation of experiments in terms of eEDM, MQM, NSM, etc. requires knowledge of the magnitude of corresponding molecular parameters such as effective electric field acting on the eEDM which cannot be measured and this is the task for modern relativistic quantum chemistry methods.

We use a method, which allows one to significantly simplify the relativistic treatment of such characteristics. This approach includes relativistic correlation calculation of valence electronic structure using the generalized relativistic pseudopotential approach followed by the non-variational restoration of four-component electronic structure in the vicinity of heavy-atom nucleus. We show [1] that this method can be efficiently combined with the direct 4-component Dirac-Coulomb-Breit approach to consider contributions of the (excluded from pseudopotential calculations) inner-core electrons, remove uncertainties due to approximate restoration procedure and treat high order correlation effects up to the coupled cluster method with single, double, triple, and perturbative quadruple amplitudes. In the report the status [1] and applications of the method to the atoms [2], molecules [1,3,5] and solids [4] most actual to search for the New physics – ThO, HfF^+, Fr, ThF^+, TaN, PbF, $PbTiO_3$, etc. are given. Calculation [5] is required for exhaustive interpretation of the experimental data by Cornell/Ye group [6].

We also show that precise relativistic methods of electronic structure calculation of molecules (finite field coupled cluster approaches) can be used to accurately extract nuclear magnetic moments from NMR experiments [7]. Applications of such methods allowed us to resolve [7] recently-established "hyperfine puzzle" [8].

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