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Effective electric field of molecules of observation experiment of electron electric dipole moment MASAHIRO FUKUDA, KOTA SOGA, MASATO SENAMI, AKITOMO TACHIBANA, Kyoto University — Heavy polar diatomic molecules are the most promising candidates for experiments of the electric dipole moment (EDM) of the electron, which is a hopeful and inexpensive probe of physics beyond the standard model. The upper bound of the electron EDM, d_e, is determined by the energy shift by the EDM, which is the product of d_e and the effective electric field $E_{\rm eff}$. $E_{\rm eff}$, which cannot be measured experimentally, must be determined by ab initio computations for each molecule based on relativistic quantum theory. Relativistic and correlation effects are essentially important for accurate computations of heavy atoms and molecules. For the former effects, the four-component Dirac equation should be solved for the inclusion of the relativistic term, such as the spin-orbit interaction, while post Hartree-Fock computations, such as configuration interaction (CI), are required for the latter effects. These two treatments consume large computational resources, and hence the value of the effective electric field has not been settled yet. In this work, we investigate the effective electric field for the electron EDM in diatomic molecules such as YbF, which is a representative one for experiments of the electron EDM.

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