RIGOROUS RELATIVISTIC METHODS FOR ADDRESSING $\mathcal{P}$- AND $\mathcal{T}$-NONCONSERVATION IN HEAVY-ELEMENT MOLECULES

TIMO FLEIG, *Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier Toulouse 3, Toulouse, France*.

A new and rigorous method for accurate ab-initio calculations of the electron electric dipole moment $\mathcal{P},\mathcal{T}$-odd interaction constant is presented. The approach uses string-based Configuration Interaction wavefunctions[a] and Dirac four-component spinors as one-particle basis functions, and the $\mathcal{P},\mathcal{T}$-odd constant is obtained as an expectation value over these correlated wavefunctions. The method has been applied to the HfF^+ molecular ion to determine spectroscopic constants for four low-lying electronic states. For one of these states ($\Omega = 1$) we have determined a new accurate benchmark value[b] for the effective electric field $E_{\rm eff}$ correlating 34 valence and outer atomic core electrons and using wavefunction expansions with nearly $5 \cdot 10^8$ coefficients. For the $\Omega = 1$ state of the ThO molecule the first ab-initio result for the electron EDM interaction constant is presented.
Aspects of modern all-electron relativistic many-body approaches applicable to both atoms and molecules will be discussed, including perspectives for the treatment of other interesting candidate systems and $\mathcal{P}$- or $\mathcal{P},\mathcal{T}$-non-conserving effects in molecular systems.

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[b] T. Fleig and M. K. Nayak *Phys. Rev. X* **XXX**, XXXX (submitted).