

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

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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_{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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^bT. Fleig and M. K. Nayak *Phys. Rev. X* **XXX**, XXXX (submitted).