

THEORETICAL ANALYSIS OF LAWRENCIUM FLOURIDE ION AS A PROMISING CANDIDATE FOR ELECTRON ELECTRIC DIPOLE MOMENT SEARCHES

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Diatomic heavy polar molecules as well as molecular ions have proved to be very good candidates for table-top experimental searches for electric dipole moment of electron (eEDM). These experiments in combination with relativistic many-body calculations set an upper bound to the eEDM, thus probing physics beyond the Standard-Model (SM) of elementary particles. Theoretically, we can check the suitability of a molecular candidate for eEDM experiments by calculating the effective electric field (E_{eff}), permanent dipole moment (μ), and polarizing electric field (E_{pol}), as these are among the major factors that determine the experimental sensitivity of the molecule. The production of radioactive elements like lawrencium opens up the possibility of performing eEDM experiments with molecules having radioactive atoms. In this abstract, we focus on lawrencium flouride ion and its potential for probing new physics beyond the SM via the eEDM. To ensure the stability of the molecule, we obtained the equilibrium bond length of LrF^+ from the minima of the potential energy curve (PEC), and we also showed how the PEC depends on the choice of basis sets. As E_{eff} is entirely relativistic in origin, relativistic calculations are required to obtain it. We report the values of E_{eff} and μ of LrF^+ calculated at Dirac-Fock level, using quadruple-zeta basis. Our calculated Dirac-Fock level value E_{eff} of LrF^+ is 213.6 GV/cm, which is two times larger than that of HgF^a , and approximately nine times larger than that of the ionic candidate $\text{HfF}^+{}^b$, thus suggesting larger experimental sensitivity. Inclusion of correlation effects to the properties by performing calculations using the relativistic coupled-cluster (RCC) method is underway. We propose a molecular ion trap procedure to confine the molecules for performing eEDM experiment with LrF^+ ion, as trap experiments would give larger coherence time compared to beam experiments, thus improving experimental sensitivity.

^aV. S. Prasanna, A. C. Vutha, M. Abe, and B. P. Das, Phys. Rev. Lett. 114, 183001 (2015).

^bW Cairncross et al, Phys. Rev. Lett. **119**, 153001 (2017).