Proposition de Stage M2

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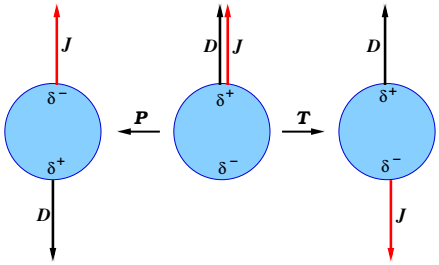
Titre: **In search for the electric dipole moment of the electron: Investigation of effective electric fields in candidate molecular systems**

The Standard Model (SM) of elementary particle physics is not the ultimate theory of the universe. Important postulated extensions to the SM (such as supersymmetric extensions, GUT's etc.) require the existence of permanent electric dipole moments (EDM) of elementary particles in the leptonic sector of matter, for example of electrons [1]. The SM predicts the electron EDM to be as small as $\approx 10^{-38}$ e cm. However, most extensions to it predict the value of the electron EDM to be many orders of magnitude larger, up to $\approx 10^{-26}$ e cm. Such values reach into the measurable range of today's modern experiments. The most promising "environment" for measuring an electron EDM is various kinds of polar diatomic molecules containing a heavy atom.



The interaction of an electron's EDM $\vec{D}$ with an electric field at it's position is necessarily parity ($\mathcal{P}$) and time-reversal ($\mathcal{T}$) violating ($\mathcal{P},\mathcal{T}$-odd). Such an interaction has so far not been observed in nature. The corresponding Hamiltonian operator has recently been implemented [2] into a powerful and general relativistic electronic-structure method [3] for atoms and molecules which is part of the `Dirac11` program package [4].

The work to be carried out in this intership concerns the search for suitable and perhaps promising candidate diatomic molecules for finding an electron EDM (such as PtH^+, HfH^+, WC, and others). The studies encompass molecular relativistic electronic structure calculations on low-lying electronic states of these molecules and the calculation of the effective internal electric fields (E_{eff}) coupling to the postulated EDM of the electron. E_{eff} is an important quantity connecting directly with the experimental measurements carried out by various groups worldwide.

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[1] E D Commins. Electric Dipole Moments of Leptons. *Adv. Mol. Opt. Phys.*, 40:1, 1999.
[2] 2012. Timo Fleig and Malaya K. Nayak, *Phys. Rev. Lett.*, to be submitted.
[3] S Knecht, H J Aa Jensen, and T Fleig. Large-Scale Parallel Configuration Interaction. II. Two- and four-component double-group general active space implementation with application to BiH. *J. Chem. Phys.*, 132:014108, 2010.
[4] DIRAC, a relativistic ab initio electronic structure program, Release DIRAC11 (2011), written by R. Bast, H. J. Aa. Jensen, T. Saue, and L. Visscher, with contributions from V. Bakken, K. G. Dyall, S. Dubillard, U. Ekström, E. Eliav, T. Enevoldsen, T. Fleig, O. Fossgaard, A. S. P. Gomes, T. Helgaker, J. K. Lærdahl, J. Henriksson, M. Iliaš, Ch. R. Jacob, S. Knecht, C. V. Larsen, H. S. Nataraj, P. Norman, G. Olejniczak, J. Olsen, J. K. Pedersen, M. Pernpointner, K. Ruud, P. Sałek, B. Schimmelpfennig, J. Sikkema, A. J. Thorvaldsen, J. Thyssen, J. van Stralen, S. Villaume, O. Visser, T. Winther, and S. Yamamoto (see http://dirac.chem.vu.nl).