



国立研究開発法人理化学研究所 仁科加速器研究センター
第236回 RIBF核物理セミナー
RIKEN Nishina Center for Accelerator Based Science
The 236th RIBF Nuclear Physics Seminar

Relativistic quantum chemistry and recent applications to physics and chemistry

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Relativistic effects in chemistry are important when molecules contain heavy atoms. This is because the electrons close to the heavy nucleus can travel rapidly, comparable to the light speed. The relativistic effects increase with atomic number Z , proportional to about Z^2 , and they provide two important features. One feature is the contraction and stabilization of s and p orbitals. Because of the contractions of s and p orbitals, d and f orbitals are expanded and destabilized in many electronic systems. The other is the spin-orbit interaction, namely spin and angular momentum coupling. The spin-orbit interaction provides intersystem crossing of chemical reactions and phosphorous emission, for example. In my talk, I will introduce some known relativistic effects in chemistry according to the review by Pykko ("Relativistic effects in structural chemistry", Chem. Rev. 88, 563-594, 1988). I will also present our recent molecular calculations for the electron's electric dipole moment (eEDM), which should be calculated based on the relativistic quantum chemistry. eEDM is attractive because it can be a probe of the Charge-Parity violation beyond the standard model. If I have time, I will talk about a finite nuclear volume effect in

* The talk will be given in English language..

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