



ID de Contribution: 50

Type: Non spécifié

Enhancement of parity-violation in chiral molecules and the origin of homochirality in nature

It has been theoretically shown that the integrated value of electron chirality density over the whole molecule is generally a nonzero value. The reaction rate of weak interactions is higher in one enantiomer than in the other due to the different number of left-handed electrons between the enantiomers. From this fact, a theory for the origin of homochirality, which is the enantiomeric excess in nature, has been proposed from the viewpoint of Electron Chirality in Chiral Molecules (ECCM).

The parity-violating energy difference (PVED) between the enantiomers of a chiral molecule is caused by the Z boson exchange between electrons and nucleons, and is proportional to the difference in electron chirality at the nuclear positions between the enantiomers. The PVED has not been observed yet experimentally because of its small value. We found numerically that the PVED is significantly enhanced in several electronic excited states for chiral molecules. To explain this enhancement of the PVED, we proposed a hypothesis named the cancellation breaking enhancement (CBE). CBE can explain the enhancement of the PVED in the first electronic excited state by focusing on the imbalance of the cancellation of contributions between molecular orbitals to the PVED.

In this study, we numerically show that not only PVED but also ECCM increases in the electronic excited states of chiral molecules. Using the CBE hypothesis, the ECCM enhancement is compared to the PVED enhancement.

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Classification de Session: Poster session

Classification de thématique: No track