

Enhancement of the parity-violating energy in chiral molecules (#4)

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“The parity-violating energy difference (PVED) between the enantiomers of a chiral molecule is caused by the Z boson exchange between electrons and nucleons. PVED is proportional to the difference in electron chirality density between the enantiomers at the nuclear positions. PVED has not yet been observed experimentally.

The integral value of the electron chirality density generally has a non-zero value in chiral molecules (Electron Chirality in Chiral Molecules; ECCM). A theory focusing on ECCM has been proposed for the origin of homochirality, which is an excess of enantiomers in nature.

We found by relativistic quantum chemical calculations that the PVED and ECCM can be significantly enhanced in some electronic excited states for chiral molecules, H₂X₂ (X=O, S, Se, Te), CHFClBr, CHFClI, and CHFBrI. This may provide new hints for observing undiscovered PVED in experiments. The behavior of ECCM was significantly different from that of PVED. Contributions from each molecular orbital to PVED and ECCM cancel each other out and become very small in the ground state. Focusing on this cancellation mechanism, we explained that PVED and ECCM are enhanced due to the cancellation breaking by electron excitation (Cancellation Breaking Enhancement; CBE).”

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