Multi-slit-type interference in carbon 2s photoionization of polyatomic molecules

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A recent study on the inner-valence MOs of a series of simple hydrocarbons with two centers has shown that the interference in coherent emission of photoelectrons from these equivalent centers represents the microscopic analogy of the Young's double-slit experiment [1]. This type of interference is related to both electronic and geometrical structure.

In the present work, we extend this research line and we enlighten the first evidence of the multi-slit-type interferences in the C 2s photoionization of several polyatomic molecules: propane, n-butane, isobutane and methyl peroxide. A more complex pattern is observed due to molecular orbital delocalization, blurring the distinction between interference and diffraction. The potential to extract geometrical information is emphasized, as a more powerful extension of the EXAFS technique.

We demonstrate that from the multi-slit interference patterns quantitative conformational analysis, generally outside the capability of photoionization studies, can be addressed, namely the determination of the relative weight of conformers in long-chain hydrocarbons and in a heterosystem (dimethylperoxide).

The experimental results are compared with the theoretical predictions by density functional theory (DFT) calculations. Cross-section calculations have been performed with the linear combination of atomic orbitals (LCAO) B-spline code [2], which provides an accurate solution of the DFT (Kohn-Sham) Hamiltonian for bound and continuum states.

References

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