

Abstract Submitted
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Core-Hole Molecular Frame X-Ray Photoelectron Angular Distributions as Molecular Geometry Probes CYNTHIA TREVISAN, California Maritime Academy, JOSHUA WILLIAMS, ADRIAN MENSSEN, University of Frankfurt, THORSTEN WEBER, THOMAS RESCIGNO, Lawrence Berkeley National Laboratory, CLYDE MCCURDY, University of California, Davis, ALLEN LANDERS, Auburn University — We present experimental and theoretical results for the angular dependence of electrons ejected from the core orbitals of ethane (C_2H_6) and tetrafluoromethane (CF_4) in an effort to understand the origin of the imaging effect by which the molecular frame photoelectron angular distributions (MFPADs) for removing an electron from a $1s$ orbital effectively image the geometry of a class of molecules. At low energies, our calculations predict the same imaging effect in C_2H_6 previously found in CH_4 , H_2O and NH_3 . By contrast, in experiment and calculations CF_4 displays an anti-imaging effect, whereby the electron ejected by core photoionization has the tendency to avoid molecular bonds, if averaged over directions of polarization of the incident X-ray beam. Our measurements employ the COLTRIMS method and the calculations were performed with the Complex Kohn Variational method.

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