Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Detection of Core Hole Localization in X-ray Photoionization[1]
CYNTHIA TREVISAN, California State University Maritime Academy, CLYDE MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory, THOMAS RESCIGNO, Lawrence Berkeley National Laboratory — In the quest to find further evidence of the core hole localization phenomenon we recently found in CF_4, we present *ab initio* calculations of molecular frame photoelectron angular distributions of electrons ejected from the core orbitals of the fluorine K-edge of various isomers of difluoroethylene ($C_2H_2F_2$). In the case of CF_4, the probability of removing a core electron from any of the four F atoms is the nearly the same for all directions of photoejection of the electron. However, we found that for a particular decay channel, detecting an F^+ ion makes the probability of having this ion be the atom that was core ionized nearly unity, because of a chemical effect related to the electronegativity of fluorine. $C_2H_2F_2$ has two symmetry-equivalent fluorine atoms. Our work explores the extent to which the localization of core holes also takes place on one of two of the fluorine equivalent atoms following X-ray photoionization and is clearly visible in an experiment that averages around the axis of recoil of ion fragments after Auger decay.

[1]U.S. DOE, Office of Science, WDTS

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Date submitted: 28 Jan 2017 Electronic form version 1.4