

Abstract Submitted
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Interatomic Coulombic Decay (ICD) in deep inner-shell vacancy cascades¹ D. RAY, R.W. DUNFORD, S.H. SOUTHWORTH, E.P. KANTER, B. KRAESSIG, L. YOUNG, D.A. ARMS, E.M. DUFRESNE, D.A. WALKO, X-Ray Science Division, Argonne National Laboratory, O. VENDRELL, S.-K. SON, R. SANTRA², Center for Free-Electron Laser Science, DESY, Germany — The photoionization of an inner-shell electron in a heavy atom triggers a vacancy cascade with the emission of x-ray fluorescence and Auger electrons leading to its final charge states. If the atom is part of a molecule or cluster, the decay process may involve removal of the valence electrons on the neighboring atoms thereby forming several charge centers and resulting in the Coulomb explosion of the system. This phenomenon in molecules where the valence electrons on the neighboring atoms play a significant role in the decay process is called Interatomic Coulombic Decay (ICD) [1]. The focus of this work is to explore the ICD effect in XeF₂ [2] following K-shell ionization of the Xe atom near 34.5 keV. We compare the total charge produced following Xe K α or K β fluorescence decay from atomic Xe and from Xe in XeF₂ molecules. We present both experimental and calculational evidence that the fluorine atoms get involved in the decay process and the molecules start undergoing structural changes during the vacancy cascade.

[1] L. S. Cederbaum et al., Phys. Rev. Lett. **79**, 4778 (1997).

[2] C. Buth et al., J. Chem. Phys. **119**, 10575 (2003).

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