

# Imaging the Cleavage of a Covalent Bond and the Subsequent Intramolecular Vibration in Gas Phase CF<sub>3</sub>I with Femtosecond Electron Diffraction

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Forming and breaking of a covalent bond is one of the most fundamental processes in chemistry. As a prototypical polyatomic molecule, photodissociation of CF<sub>3</sub>I involves in important concepts including intersystem crossing, Jahn-Teller splitting and intramolecular vibrational energy redistribution (IVR) in the photofragment [1].

Gas phase ultrafast electron diffraction (UED) is a technique pioneered by Prof. A. Zewail and a few other groups in the end of last century [2], with the promise of making atom-resolved molecular movies. However, it was until 2016 when the first molecular movie of coherent nuclear motion with both atomic spatial (sub-Å) and temporal (200fs) resolution was demonstrated by our group, employing mega-electron-volt (MeV) relativistic UED [3].

In this presentation, we present experimental study of photodissociation of the C-I bond in gas phase CF<sub>3</sub>I using MeV UED. Rich structural information that reveals the initial bond breaking dynamics as well as the subsequent vibrational motion in the photofragment are observed directly in the diffraction patterns. This work shows that MeV UED is capable of producing unprecedented details in nuclear structural dynamics, which is critical for understanding photochemical processes.

## References:

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[3] J. Yang *et al.*, Phys. Rev. Lett. **117**, 153002 (2016)