# Imaging Molecular Reactions with Atomic Resolution

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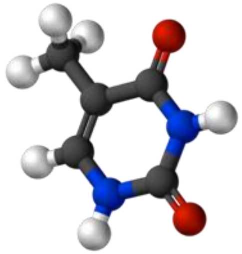
# Making a Molecular Movie

**Goal: Understand and control the conversion of light into other forms of energy at the molecular level.**

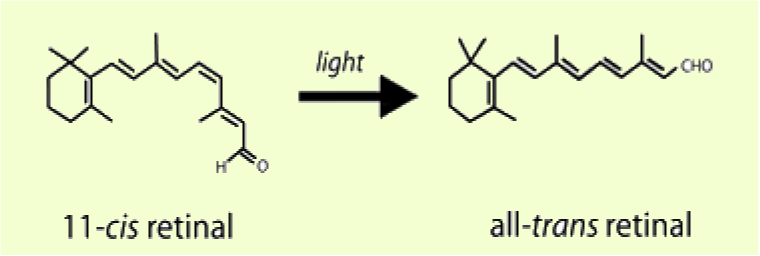
- **Light is converted into mechanical energy (vibrations) or into chemical energy through bond breaking and changes in the shape of the molecule.**

- **We need to first observe a reaction as it takes place, on the atomic scale and on ultrafast time scales.**

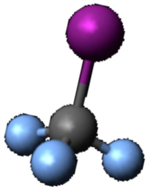
Thymine



Retinal




$CF_3I$



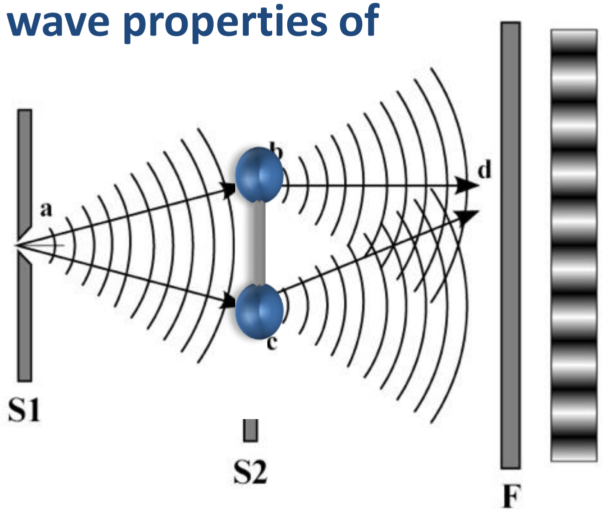
# Ultrafast and Ultrasmall

**Need very high spatial and temporal resolution to see the motion of atoms during a molecular reaction:**

- Interatomic distances ~ 1Å ($10^{-10}$ m) – 10,000 times smaller than the resolution of an optical microscope.
- Motion of atom on the scale of 200 fs ($2 \times 10^{-13}$ s) - Less than one trillionth of a second)

**Electron diffraction is sensitive to atomic structure due to the wave properties of electrons:**

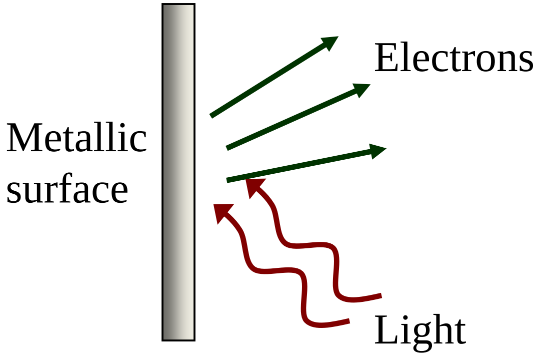
Young's double slit interference



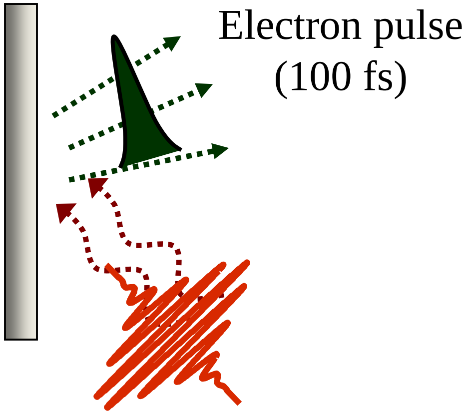

*The distance between the slits can be calculated from the frequency of the interference pattern*

# How to generate electron pulses

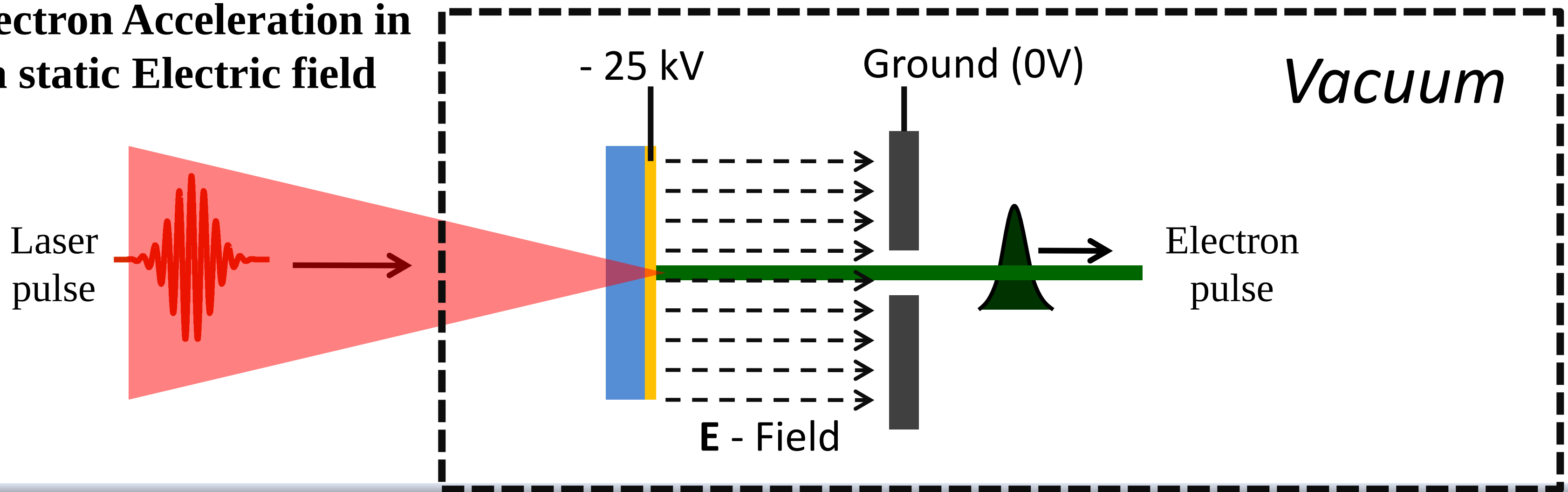
Photoelectric Effect




Electron Pulses from Laser pulses

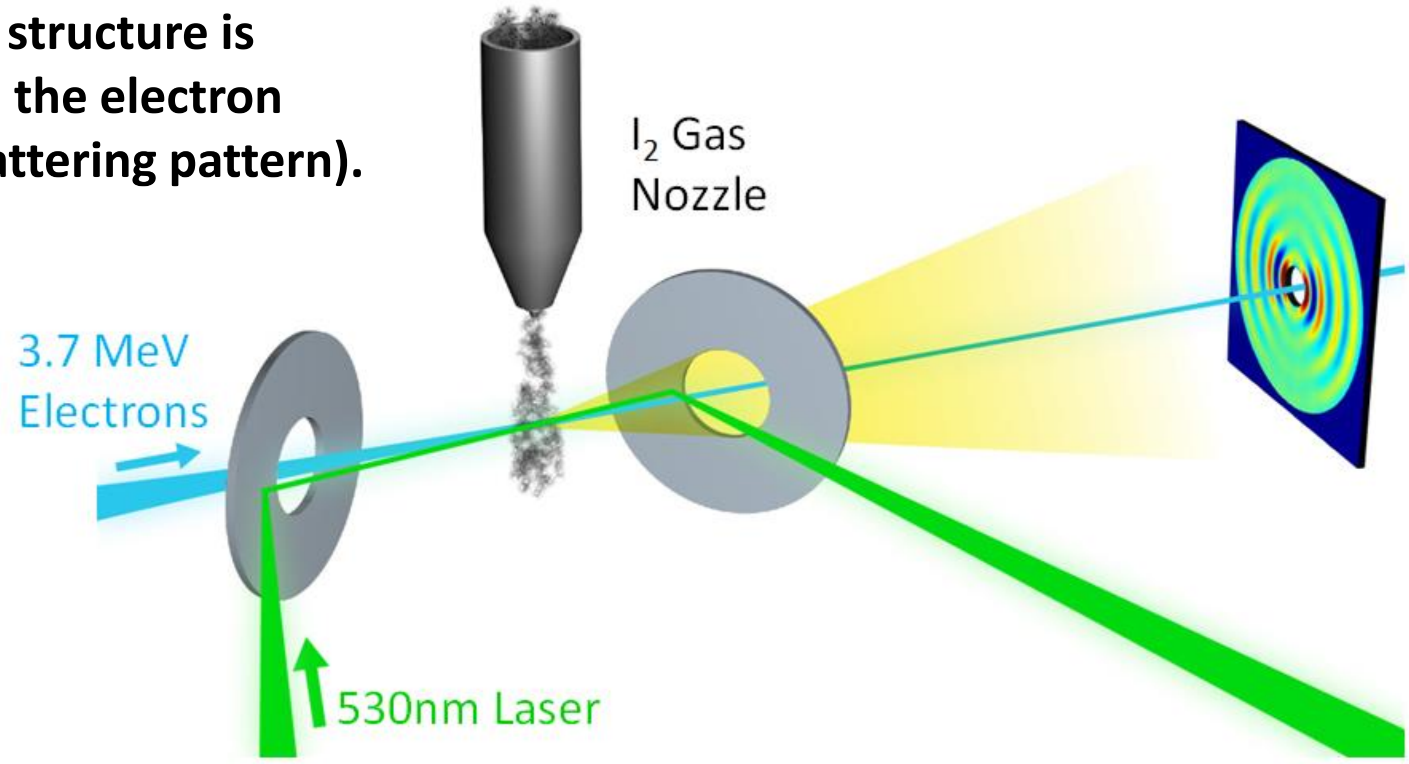



**Electron Acceleration in a static Electric field**

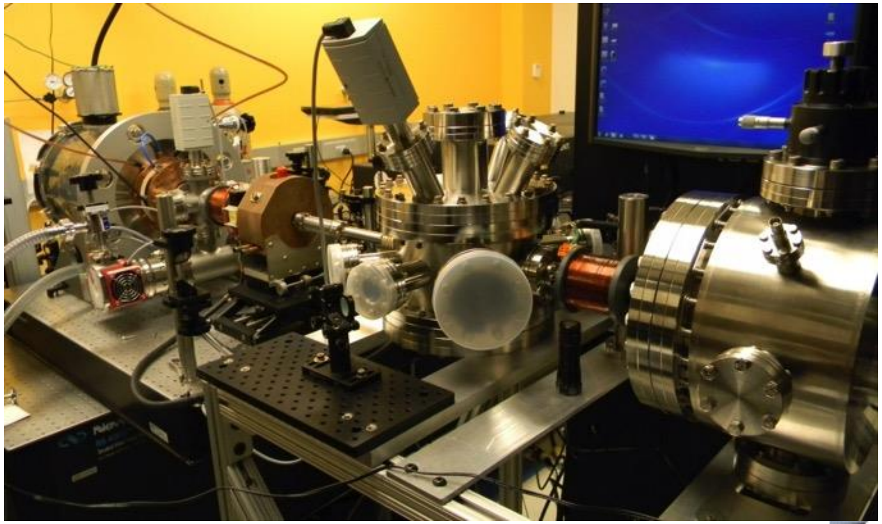


# Ultrafast Electron Diffraction

- **The target molecules are introduced in a gas beam.**
- **First the laser excites the molecules, then the electron pulse scatters from the molecules.**
- **The molecular structure is retrieved from the electron diffraction (scattering pattern).**



# Ultrafast Electron Diffraction Experiments

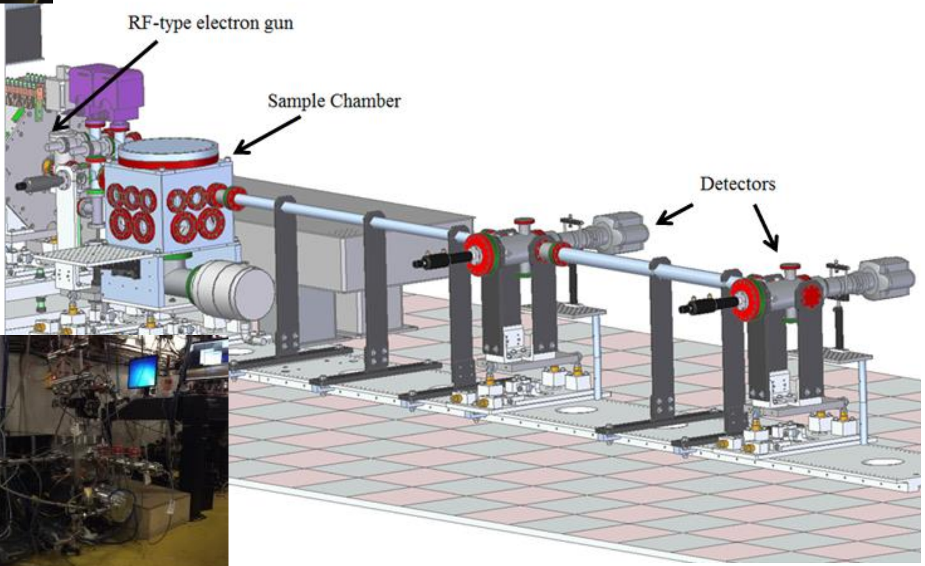


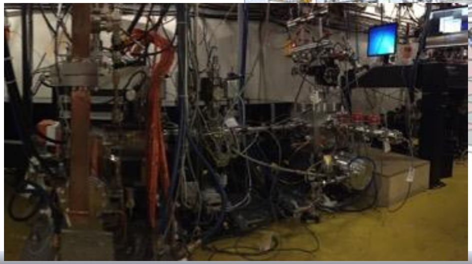
**Setup at UNL**

- **300 fs resolution**
- **Sub-relativistic energy (0.1 MeV)**
- **Table-top**

**Setup at SLAC National Lab**

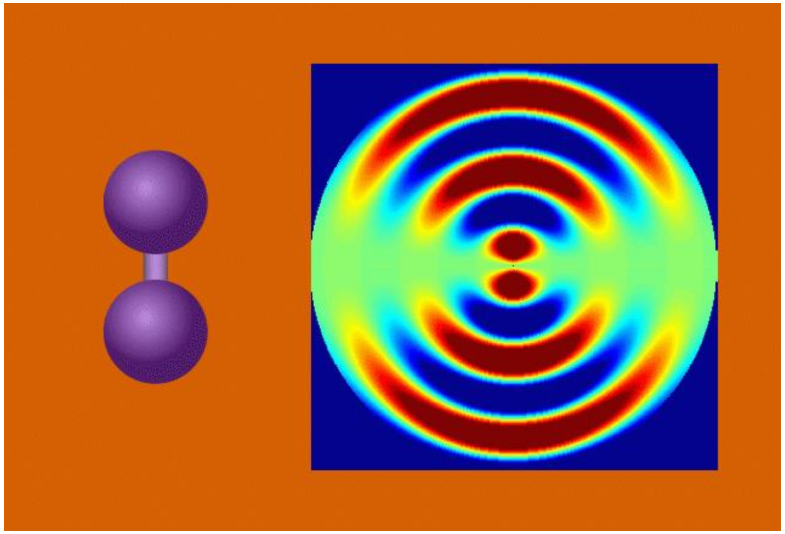
- **100 fs resolution**
- **Relativistic energy (4 MeV)**



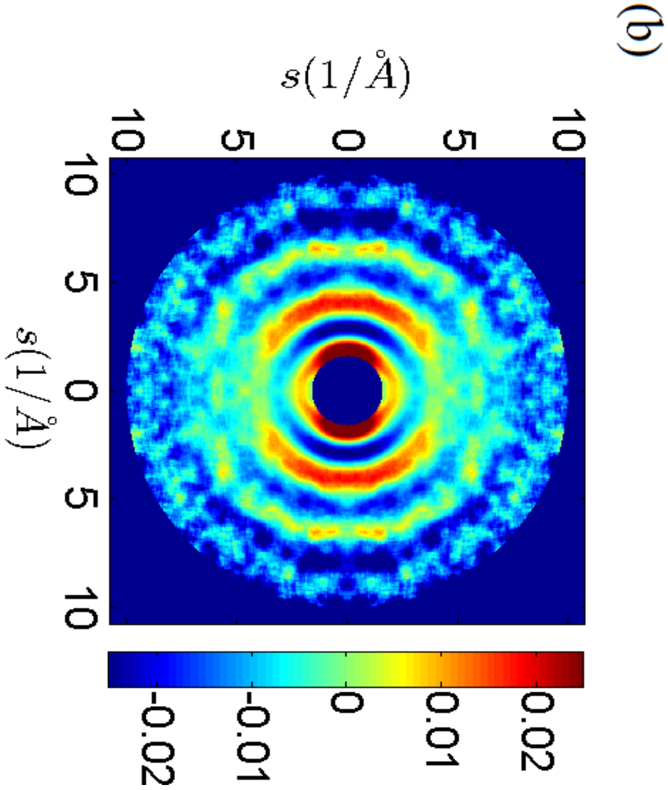
# First Molecular Movie (2016)

**Simulated diffraction from a vibrating Iodine molecule**



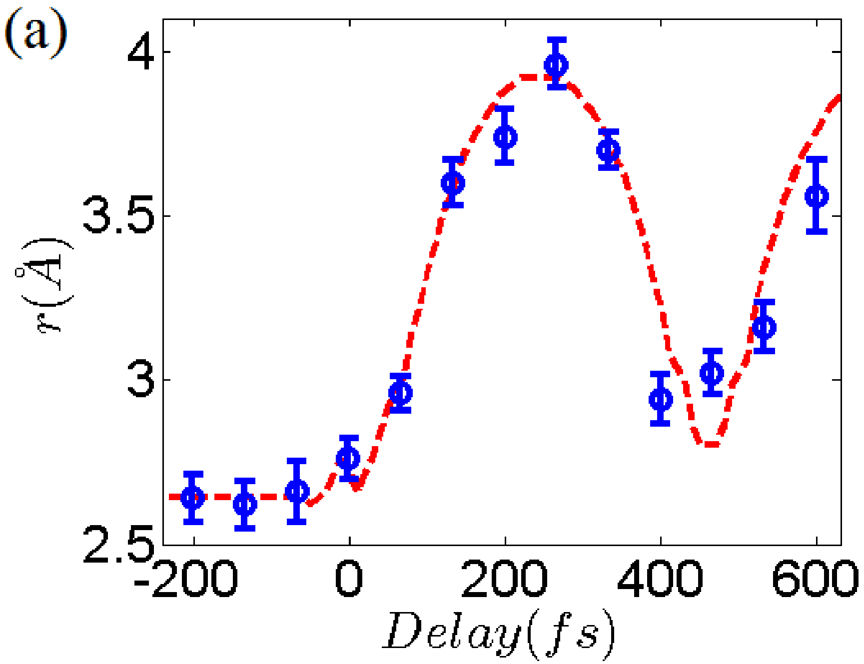
**The vibration is triggered by a femtosecond laser pulse.**

**Measured Diffraction Pattern**



# Following the motion

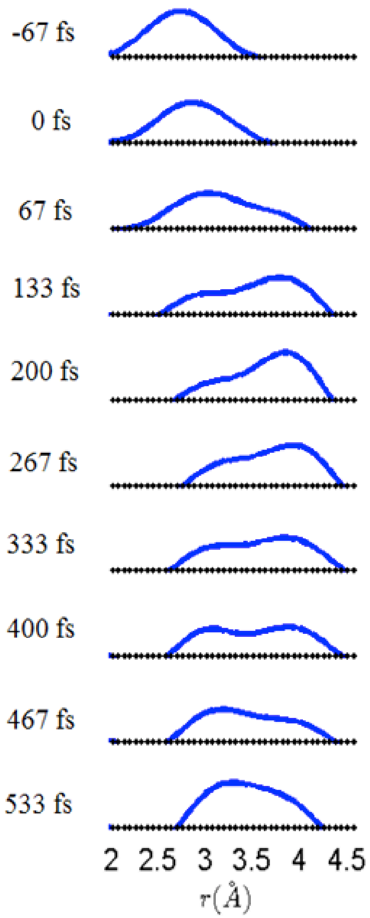
**Captured vibrations with atomic resolution**




**Blue dots: Data**

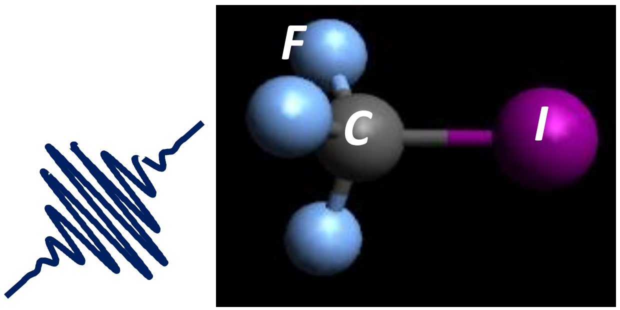
**Red line: Theory**

**Changes in the shape of the moving wavepacket can also be measured.**
**This is a purely quantum mechanical effect.**

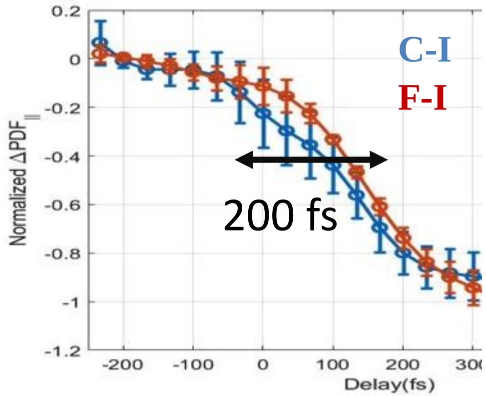


# Imaging the Breaking of a Chemical Bond (2017)

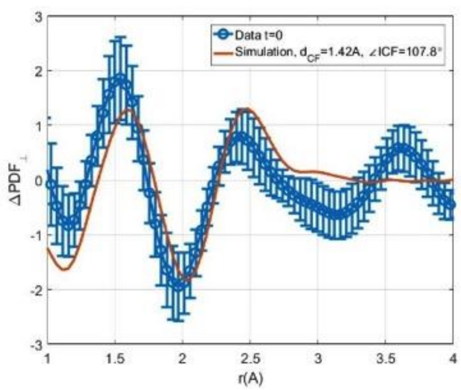
After absorbing light, the Carbon-Iodine chemical bond breaks.




$CF_3I$ Molecule

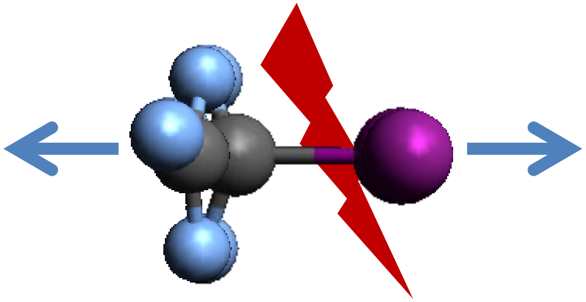



The bond breaks in less than 200 fs.



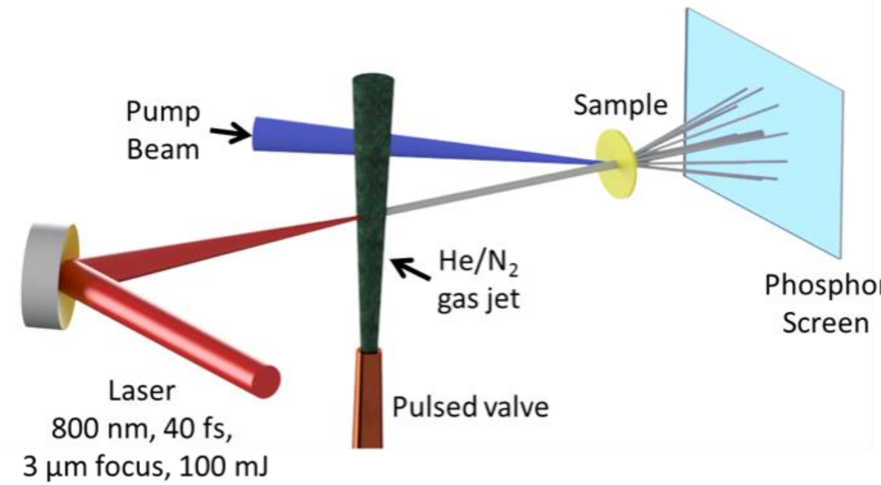

The heavy Iodine atom pushes the carbon atom away and the structure of the $CF_3$ fragment becomes more planar.

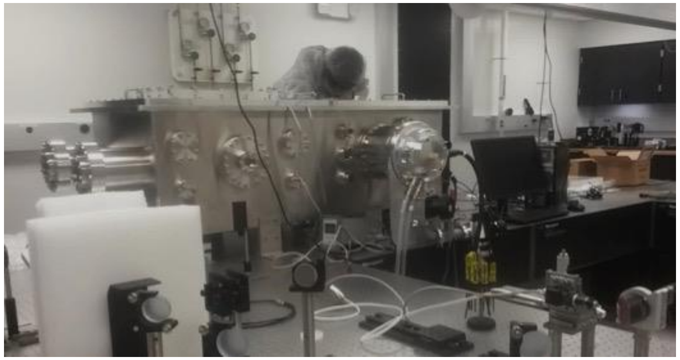
**The reaction as captured in the experiment:**



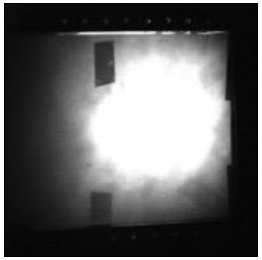
# Relativistic Electron Diffraction at UNL

## High energy (MeV) electron pulses generated with the Archimedes laser at the Extreme Light Core Facility (ELCF)

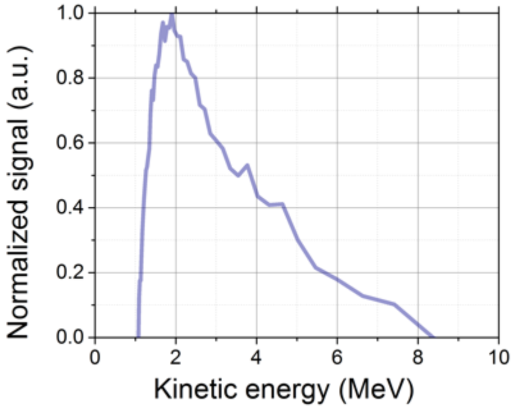


### Electron Beam



### Electron Energy




First successful experiments to generate highly charged pulses in 2017:

- More than 1 billion electrons per pulse (1000 x more than with standard methods).
- Energies around 1-3 MeV are ideal for diffraction.

# Summary

- First atomically resolved movies captured with ultrafast electron diffraction.

- Laser accelerated electron pulses are promising for capturing the interaction of matter with intense laser fields where the image must be captured in a single shot.

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# Acknowledgements

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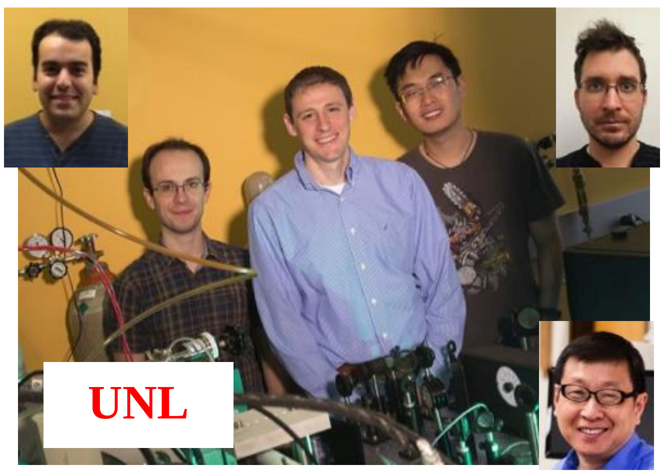


**UNL collaborators**

Matthias Fuchs

Brad Shadwick

Donald Umstadter

**External collaborations**

Xijie Wang, Mike Minitti (SLAC National Lab)

Markus Guehr (Potsdam University – Berlin)

Thomas Wolf, James Cryan, Ryan Coffee (Stanford Pulse Institute)

Derek Wann (University of York).

Todd Martinez (Stanford University).