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Ultrafast Photoelectron Circular Dichroism Changes in 1-Iodo-2-Methylbutane

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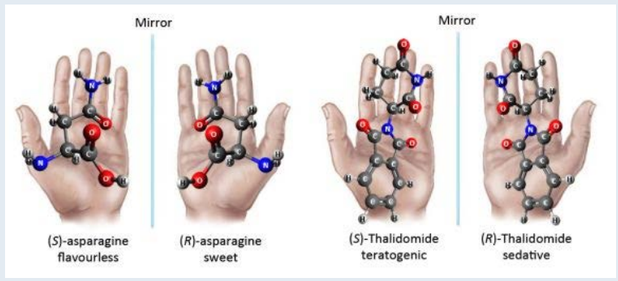
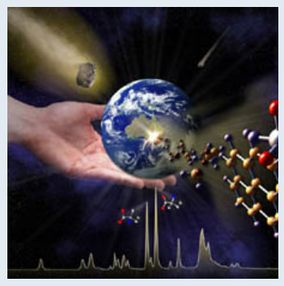
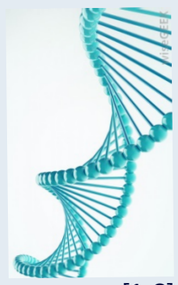
Goal of the FLASH-Experiment

Evaluate the method of PECD as a tool for chiral recognition during ultrafast dynamics as well as to understand and eventually control photo-induced processes in chiral systems.

Motivation of the Scientific Agenda







[1-3]

- All known living tissue is homochiral → Human bodies are chiral receptors.
- Hundreds of billions of $ are spent annually for controlling the chirality of e.g. pharmaceuticals.
- PECD is a very sensitive method to sense and study chirality.

Aims of the Experiment

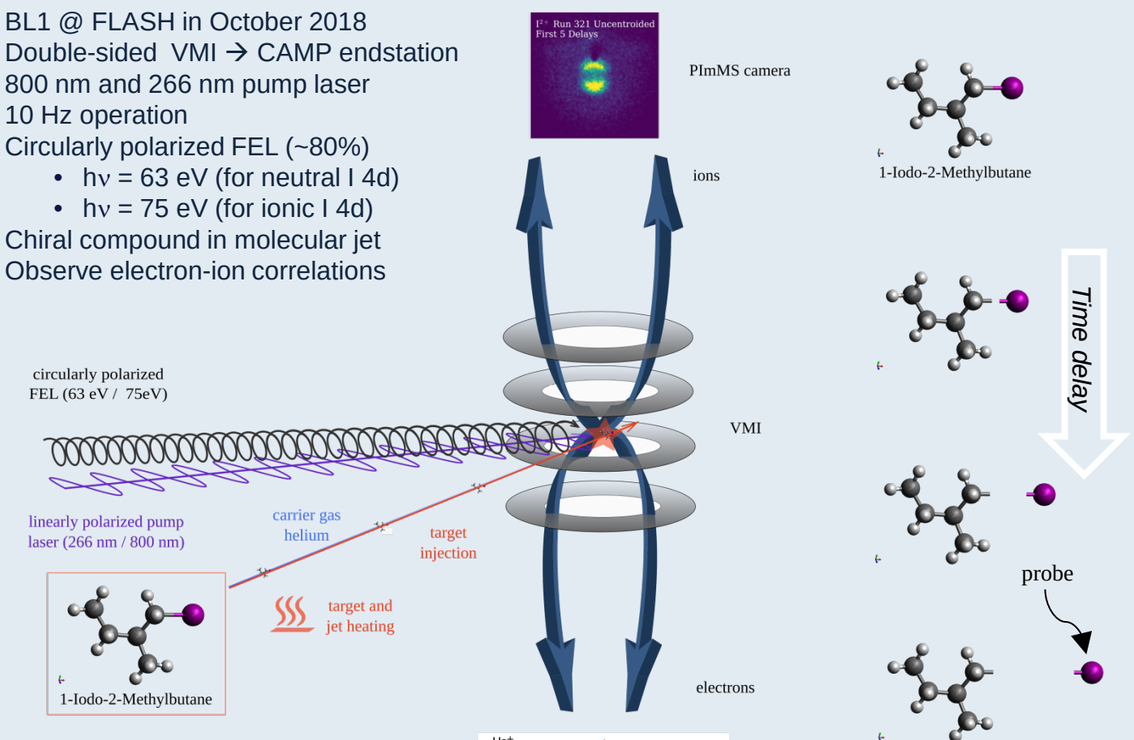
a) Characterization of the chiral target and its dissociation dynamics for the neutral and charged iodine fragment as 'observer atom'. For different fragmentation channels and time delays (0 to -1500 fs) for left- and right circularly polarized XUV radiation and 3 different target forms, i.e. S-enantiomer, R-enantiomer, and racemic mixture.
Method: electron and ion velocity map imaging (VMI) spectroscopy.

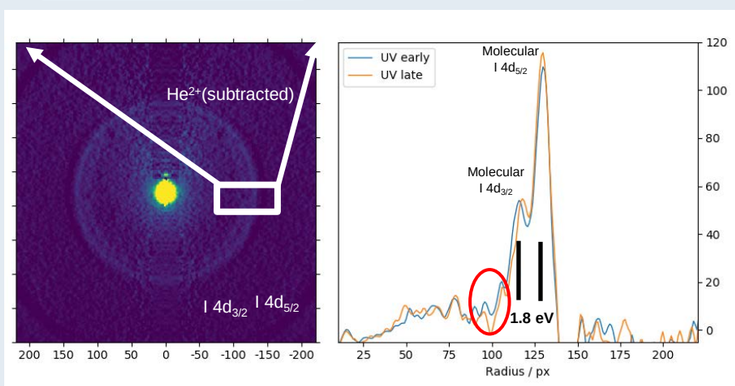
b) Obtaining PECD at the iodine $4d_{3/2}$ and $4d_{5/2}$ states.

c) Determination of the time-resolved photoelectron circular dichroism (TR-PECD) at the iodine 4d edge of the atomic iodine fragment.

Experimental Overview

- BL1 @ FLASH in October 2018
- Double-sided VMI → CAMP endstation
- 800 nm and 266 nm pump laser
- 10 Hz operation
- Circularly polarized FEL (~80%)
  - hν = 63 eV (for neutral I 4d)
  - hν = 75 eV (for ionic I 4d)
- Chiral compound in molecular jet
- Observe electron-ion correlations

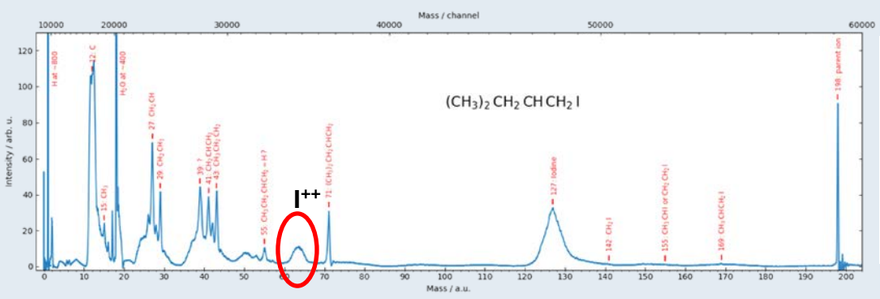




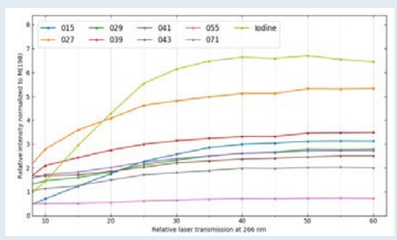
- 266 nm early by 500 fs.
- He^{2+} subtracted.
- Angle integrated electron spectra for all sources.
- Atomic iodine will be chemically shifted by ~1.6 eV [4].

Time-of-Flight Mass Spectra

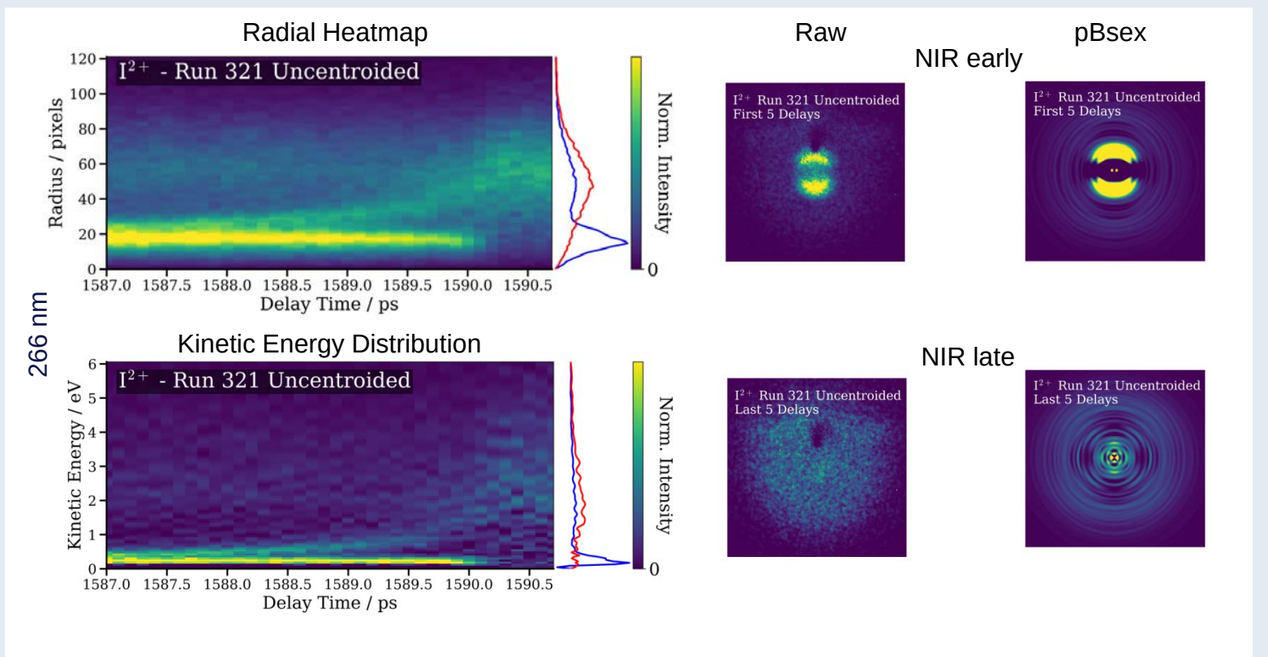
800 nm



266 nm



PImMS Data (University of Oxford – Courtesy of F. Allum)



Electron-Ion Correlations

- Differentiate atomic and molecular identities via kinetic energy of the electrons.
- Disentangle pathways that create iodine 2+ via PImMS KER maps.
- Use machine learning approaches to filter principal components and to analyze all involved correlations.
- Involve all statistics in order to obtain statistically robust forward-backward information for ‚red circle'.
- The atomic iodine $4d_{3/2}$ is the only contribution that is energetically in a ‚clean' position.

- UV early by 500 fs.
- Only electrons that come together with I^{2+} fragments.
- PECD: Up-down asymmetry in the ‚blue circle'.

Data analysis ongoing.

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