

# Recent developments towards time-resolved gas-phase electron diffraction at York

J. Pedro F. Nunes<sup>1\*</sup>, Conor D. Rankine<sup>1</sup>, Stuart Young<sup>1</sup>, Matthew S. Robinson<sup>2</sup>, Paul D. Lane<sup>3</sup>, Derek A. Wann<sup>1</sup>

<sup>1</sup> University of York, Heslington, York, YO10 5DD, UK

<sup>2</sup> University of Nebraska-Lincoln, 1400 R St, Lincoln, NE 68588, United States

<sup>3</sup> Heriot-Watt University, Riccarton, Edinburgh, EH14 4AS, UK

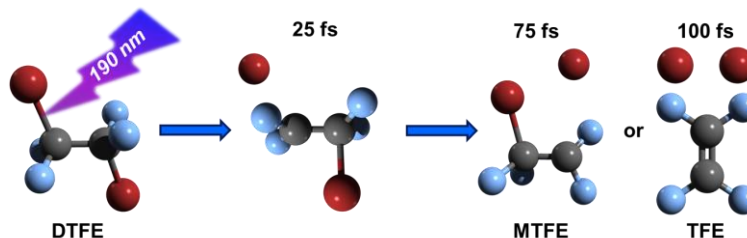
\* jpf500@york.ac.uk

An apparatus has been built to allow time-resolved electron diffraction (TRED) experiments to be performed in the UK for the first time.<sup>1,2</sup> The Wann group TRED apparatus, shown in Figure 1, employs a compact electron gun to produce short electron bunches using the third harmonic of an 800 nm Ti:Sapphire femtosecond laser focused onto a gold photocathode. These electron bunches are then accelerated across a potential of up to 100 kV towards a sample placed in a diffraction chamber.

Since its commissioning, the apparatus has been used to record time-averaged diffraction patterns for polycrystalline and gas-phase samples, examples shown in Figure 2.

In preparation for the first time-resolved experiments using the TRED apparatus, the dynamics of the photodissociation of 1,2-dibromotetrafluoroethane (DTFE) have been explored computationally. DTFE, also known as Halon2402 or Freon114B2 is used industrially as: a fire suppressor, refrigerant and leak detector, and is widely used as a building block for the synthesis of fluorinated compounds, such as tetrafluoroethyl substituted aromatics and polymers.<sup>3</sup>

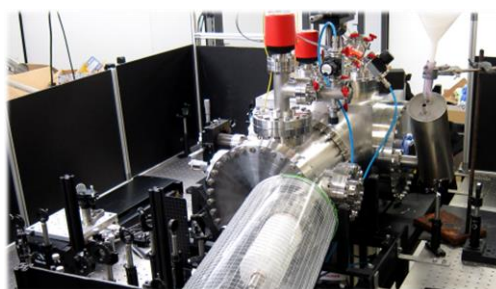
The dissociation of DTFE post-illumination by ~190 nm laser light, was studied over a period of 400 fs using CASSCF(8,6) non-adiabatic molecular dynamics. Two possible dissociation pathways have been identified, and the timescale of formation of the products, shown in Figure 3, have been determined.



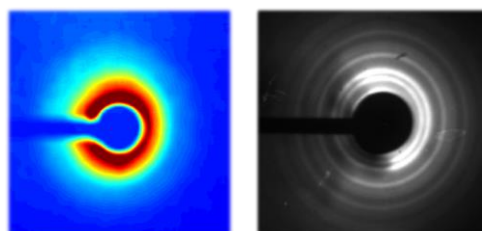
**Figure 3:** Diagram illustrating the two pathways for the dissociation of DTFE, producing tetrafluoroethene (TFE) and monobromotetrafluoroethane radical (MTFE).

## References

- (1) M. S. Robinson, P. D. Lane, D. A. Wann, *Rev. Sci. Instrum.*, **86**, 013109 (2015)
- (2) M. S. Robinson, P. D. Lane, D. A. Wann, *J. Phys. B*, **49**, 034003 (2016)
- (3) W. Dmowski, *J. Fluor. Chem.*, **142**, 6-13 (2012)



**Figure 1:** TRED apparatus at York.



**Figure 2:** Diffraction patterns recorded.