

THE UNIVERSITY of EDINBURGH School of Chemistry

Project Title

Ultrafast Structural Dynamics Imaging of Carbonyl Photochemistry

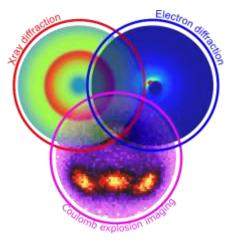
A PhD position is available in the Green Research Group at the University of Edinburgh; School of Chemistry, <u>https://www.ed.ac.uk/profile/alice-green</u>.

The PhD Studentship is fully funded for 42 months by the University of Edinburgh and covers tuition fees and an annual stipend at the UKRI rate, for 2024-25 this is £19,237 per annum. International applicants are eligible to apply.

Project Summary

Understanding the mechanisms of chemical reactions triggered by the absorption of light is critical in modelling the evolving chemical makeup of the atmosphere. The dynamics that drive photochemical reactions occur on ultrafast (~femtoseconds, 10⁻¹⁵ seconds) timescale. The latest experimental methods now can allow us to directly image the ultrafast motion of nuclei during the photochemical reactions of isolated molecules. Doing so allows us to probe the potential energy landscape which determines photochemical reaction outcomes in exquisite detail.

This PhD project will apply these emerging gas-phase experimental methods to investigate the ultrafast chemistry of small carbonyl molecules. These species are of considerable atmospheric importance as they form a substantial component of secondary organic aerosols, molecules which are emitted (by both man-made and natural processes) in large quantities. The experimental methods used include: time-resolved Coulomb explosion imaging [1], ultrafast electron diffraction [2], time-resolved X-ray scattering [3] and time-resolved X-ray spectroscopies [4]. Each method is preferentially sensitive to different aspects of the complicated dynamics of photochemical reactions, and so we aim to combine their insights to produce a more complete mechanistic picture.



It is expected that the applicant will have a strong undergraduate degree in Chemistry, Physics, or a related subject. The project will involve: ultrafast laser spectroscopy, high-vacuum experimentation, charged-particle detection and data analysis. Experience with any of these topics is useful but not essential to apply. The student will receive extensive supervision and guidance on all of these topics.

The student will join the newly-formed research group of Dr Alice Green, who started as a Lecturer in Physical Chemistry/Chemical Physics at the University of Edinburgh in 2024. As such, the student will work closely with Dr Green. During the course of the project, capabilities will be built up in the laboratory in Edinburgh, with further experiments anticipated at a number of international free-electron laser facilities. These facilities include: the European XFEL (Hamburg, Germany), the LCLS (California, USA) and SwissFEL (between Basel and Zurich, Switzerland).

References

1. Jahnke, Till, *et al.* "X-ray Coulomb explosion imaging reveals role of molecular structure in internal conversion." arXiv preprint <u>arXiv:2405.15367</u> (2024).

2. Centurion, Martin, Wolf, Thomas JA and Yang, Jie "Ultrafast imaging of molecules with electron diffraction." *Annual Review of Physical Chemistry* 73(1) 21-42 (2022); <u>10.1146/annurev-physchem-082720-010539</u>.



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3. Stankus, Brian, *et al.* "Advances in ultrafast gas-phase x-ray scattering." Journal of Physics B: Atomic, Molecular and Optical Physics 53(2), 234004 (2020); <u>10.1088/1361-6455/abbfea</u>.

4. Kraus, Peter M., Zürch, Michael, Cushing, Scott K., Neumark, Daniel M. and Leone, Stephen R. "The ultrafast X-ray spectroscopic revolution in chemical dynamics." *Nature Reviews Chemistry* 2(6), 82-94 (2018); <u>10.1038/s41570-018-0008-8</u>.

How to Apply

Interested students are encouraged to contact Alice Green with any questions before applying. Applications from all backgrounds and informal discussions on the research project are welcomed. The application should include a cover letter and CV, and should be directed by email to:

Alice Green, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. Email: alice.green@ed.ac.uk

Your cover letter should include:

- Your motivation for joining the Green Research Group
- Why your skills and experience are relevant to the position

In your CV please include details of any research you have undertaken.

The position will remain open until filled. A closing date may be added at a later date.

IMPORTANT

Before Submitting your cover letter and CV, please complete the online <u>School of Chemistry</u> <u>Equality, Diversity and Inclusion Form, entry 2025-26.</u>

The form will automatically generate a unique 'Response ID number' that you <u>must</u> include in your cover letter.

Equality and Diversity

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality.

The University has a range of initiatives to support a family friendly working environment. For further information, please see our University Initiatives website: <u>https://equality-diversity.ed.ac.uk/inclusion/family-and-carer</u>