

# Universal Approach for Solving Real-World Problems Using Quantum Dynamics: Coherent States for Molecular Simulations (COSMOS)

## Year 2 Report

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## **1 Introduction and Objectives**

The programme grant has finished the second year out of six and this report relates to work carried out over the 12 months from Oct. 2024-Sept 2025. The grant aims to develop transformative new QD simulation strategies that will uniquely deliver impact and insight for real-world applications across a range of technological and biological domains. The central objective of our programme grant is to provide a new universal methodology and suite of software to perform QD simulations of complex systems, and demonstrate the game-changing ability this would provide for the understanding of fundamental processes involved in both light-driven chemical processes and quantum technologies. The focus of the first two years has been to set up the infra-structure required to deliver the new software and support the development of new methods and their application.

Specific objectives are:

1. To develop new methods for QD simulations that span experimental, technological and biological ranges of time- and length-scales
2. To build a QD code that can be used by both experimental and computational researchers
3. To deploy our QD code to provide new insight into light-matter interaction in complex molecules and materials, demonstrating commonalities in seemingly disparate phenomena
4. To develop future quantum technology simulators, such as qubit-based quantum computers, for conventional computers
5. To provide community training in QD simulations, building new bridges across different application domains

Over the last year, 29 papers have been published with support from the grant. This includes 11 papers involving our project partners and community roadmap papers on machine learning and benchmarking quantum dynamics. The PIs have also delivered 29 talks at workshops and international conferences promoting the project and the work being done. Training workshops have been run in Spain, Germany and the UK to introduce how to run quantum dynamics calculations. Three summer students were hosted as part of the programme outreach, and the art-science collaboration that will provide a route to target non-expert audiences has been started.

## **2 Milestones for the Initial Period**

Fig. 1 shows the workplan for the first 3 years. The first year aimed to primarily set up the infrastructure required for the work to be performed. Progress for the various milestones during the second year is

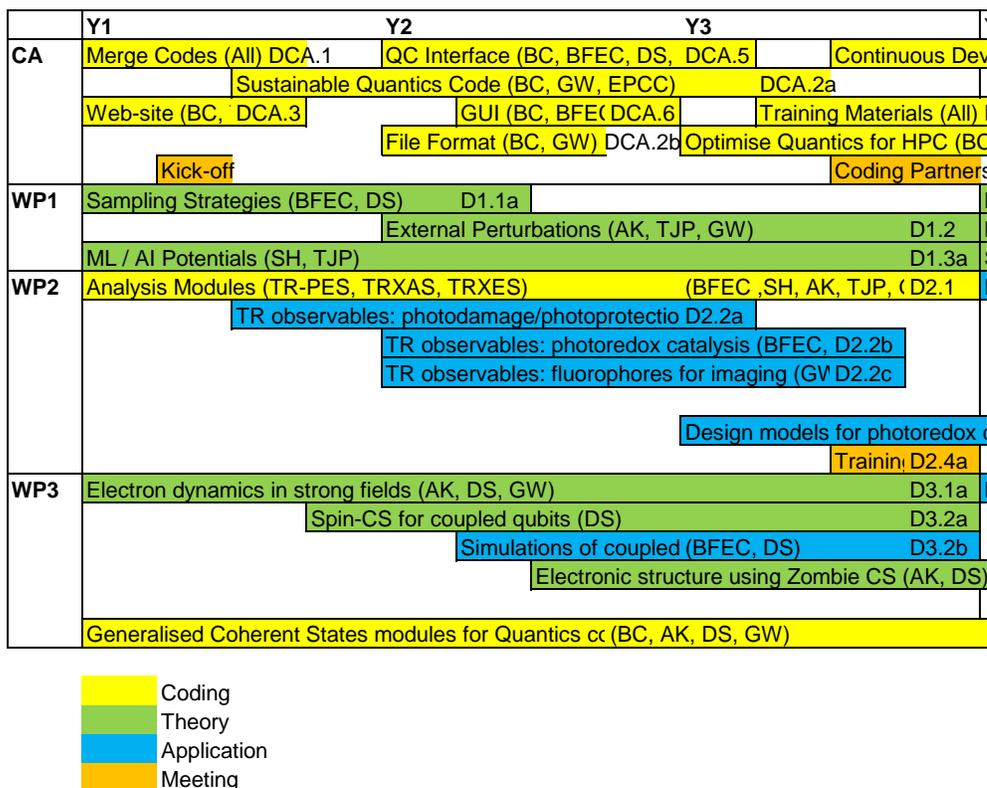


Figure 1: Planned work and activities for the first 3 years of the programme

described below and in the Appendix the health of the different projects is demonstrated.

## 2.1 Central Activity (CA). Lead: ES

### 2.1.1 Merge Codes

The aim is to bring codes together and provide the framework for collaborative development. This will be done in the community package Quantics, and controlled through a Gitlab repository.

1. The structure of the SQLite database at the heart of the direct dynamics simulations in Quantics has been finalised. A paper is in preparation to publish the format, allowing other researchers to make output compatible with Quantics.
2. The QC interface code that enables Quantics to read the information required for dynamics calculations has been further improved, with a new interface to the ORCA program. This means there are now interfaces to 12 codes.
3. The original FMS90 code (ab initio multiple spawning, AIMS) has been fully restructured and modernized by Daniel Hollas and Yorick Lassmann (Curchod group), and will be released in November

2025 as an open source code – OpenFMS. The interface between OpenFMS and Quantics is ongoing. OpenFMS will also be used as a platform for the implementation of the methods multi-configurational Ehrenfest (MCE) and ab initio multiple cloning (AIMC). developed in the Shalashilin group.

4. The Zagreb Surface Hopping Code interface with Quantics has been updated (Worth and Sanz Sanz (Madrid)) to include triplet states.

### **2.1.2 Sustainable Quantics Code**

The sustainable development will be based on the use of Gitlab which provides the main tools. A team of Quantics Maintainers has been set up to help administer the Gitlab site and oversee the work. Overall control is kept by the PI, Worth and the other maintainers are all project partners: Oriol Vendrell (Heidelberg), Cristina Sanz Sanz (Madrid), Sandra Rodriguez Gomez (Madrid).

The second strand of sustainable development is through training. It is important that developers work in the same way. To help train the COSMOS team, a Hackathon was held at Warwick 16-17 June 2025. More details are given below under Training.

Contact has been made with the Edinburgh Parallel Computing Centre (EPCC) who will be providing support for sustainable development and porting the code to HPC. A software developer will be assigned at 50% over the next 4 years, starting in Nov. 2025.

### **2.1.3 Web-site**

The COSMOS web-site now has a domain and is hosted under <https://cosmosproject.co.uk>. It is a site based on Hugoplate, a free starter template built with Hugo and TailwindCSS, designed and developed by Zeon Studio and released under the MIT code license. The website includes information about the COSMOS Team, a list of publications with minipages for each publication, latest news and events and information such as the code of conduct and ED&I. Each of these will continue to be improved and updated over the course of the project.

Work on updating and improving the Quantics web-site is still ongoing, but it is nearly ready for release. It will provide a better platform for exchange of information on the code and how to use it.

### **2.1.4 Discourse Forum**

A forum for exchange of information and questions has been set up on the Discourse platform. At present it is available only to PIs and members of the teams to test and set up. Once it has been established, it will be made open to all to provide a focus for researchers using the Quantics codes.

## **2.2 Workpackage 1. New Methods for Quantum Dynamics. Lead GW.**

The research group at Warwick (Habershon) have recently demonstrated [*J. Chem. Phys.*, **163**, 024127 (2025)] how GWP basis functions that are full-dimensional - yet follow trajectories in a lower-dimensional

space - can be used to accurately represent time-dependent wavefunctions. These so-called ‘tethered’ GWPs (t-GWPs) have the significant advantage that the extent of higher-dimensional space spanned by each basis function does not ‘shrink’ as system dimensionality/complexity increases; this approach helps to circumvent the well-known ‘curse of dimensionality’ that typically demands an exponentially-increasing GWP basis-set size as the number of degrees-of-freedom under study increases. The novel t-GWP basis set - and related methodology - is now being integrated into the central Quantics code. In particular, integrating t-GWP basis functions with ML strategies such as kernel ridge regression (KRR) - already well demonstrated in the context of both MCTDH and vMCG simulations - will enable a ‘direct dynamics’ variant of GWP-based dynamics, while hooking t-GWPs into the diabatisation strategies implemented in Quantics will support new non-adiabatic simulations. Finally, we note that a new PhD student [Adam O’Hare, Warwick, 2025 - 2029] associated with the COSMOS project will initially focus on deploying t-GWPs and similar lower-dimensional strategies as part of vMCG calculations coupled to ML models for direct dynamics.

The research group at Oxford (Kirrander) continued their work on algorithms for the analysis and interpretation of quantum molecular dynamics simulations. They introduced a new clustering algorithm that is particularly suitable for the varied and multidimensional output generated by trajectory-based simulations of photoexcited dynamics [*J. Chem. Theory Comp.*, **21**, 5789 (2025)]. The algorithm approximates the underlying probability density function using variable kernel density estimation, with local maxima corresponding to cluster centers. Each data point is then assigned to one of the maxima by employing a maximization procedure. Finally, clusters artificially separated by minor fluctuations in the probability density are merged. Importantly, algorithm does not require parameter-tuning, which ensures flexibility and reduces the risk of bias. The algorithm is currently evaluated on a larger set of relevant molecular simulations, and once this is finished, this methodology will be interfaced with the simulation methods already available in QUANTICS.

The COSMOS Team (and a large number of its partners) participated to a Roadmap article establishing the best practices to benchmark methods for nonadiabatic molecular dynamics and establish a timeline for the development of a series of standardized benchmark systems. These benchmark systems will be available in Quantics. Worth and a number of project partners also met at a Cecam workshop in Zaragoza (Sept 2-5, 2025) on benchmarking. This provided a framework for developing the benchmarks required to validate new simulation methods.

In the Worth group (UCL), the focus has been on developing fitting methods to provide potential energy surfaces from the databases obtained from DD-vMCG calculations which can be used in grid-base QD. This is required to provide proper benchmarking of the Gaussian Wavepacket methods under development. Three main strands are under development. The first, together with the Habershon group, is to use Gaussian Processes Regression which provides surfaces the the form of a sum of Gaussian functions. The second is using neural nets to fit surfaces as a sum of exponential functions. The third, together with Daniel Pelaez Ruiz (Paris Sud), is to use a novel machine learning approach to provide multi-dimensional surfaces as a tensor decomposition of polynomials.

### **2.3 Workpackage 2. Quantum Dynamics in Chemistry. Lead: BFEC.**

In early February, the COSMOS consortium met online to discuss the progress of Workpackage 2. The Penfold group highlighted their recent work on the development of LVC models for the design of rigid planar charge-transfer molecules to be used in TADF. These models can be developed around known

molecular systems and used to predict specific properties for the preparation of new molecules. The Worth group has been working on the development of models for benchmarking strategies, focusing on different strategies to obtain potential energy surfaces (and compare their outcome). The Shalashilin group highlighted their recent applications of nonadiabatic molecular dynamics to electron-impact generated triplet states (in plasma), a process of central importance for the microelectronic industry. The simulations performed in the Shalashilin group indicate that nonadiabatic molecular dynamics can provide triplet dissociation channels and product quantum yields, of central importance to characterize the use of electron-impact chemistry in industry. Leeds group published a paper describing newly introduced electrophore model of dissociation after electron impact in the *Journal of Vacuum Science and Technology* to reach the community of scientists and engineers working in the area of plasma technologies for microelectronics. This paper represents a COSMOS effort to make an impact beyond chemistry and the plasma chemistry project of Leeds group is in collaboration with industry. The Curchod group studied the photophysics of photoredox catalyst called DDQ, in collaboration with laser spectroscopists (Orr-Ewing group, Bristol) and a synthetic group (Lennox group, Bristol). The interest for DDQ has recently grown in the synthetic chemistry community thanks to the ability of this molecule to perform proton-coupled electron transfer to functionalize organic molecules. Calculations confirmed an ultrafast intersystem crossing event for the DDQ molecule, and its stability in a low-lying triplet state, allowing for further bimolecular reactivity.

The Bristol team (Curchod) wrote an article for *Accounts of Chemical Research* discussing the importance of adequately selecting initial conditions for trajectory-based nonadiabatic molecular dynamics simulations. This work aligns with the development of approaches to simulate time-resolved observables.

The Newcastle team (Penfold) published an article in *The Journal of Physical Chemistry Letters* that combined theory and experiment to unravel the ultrafast quantum spin dynamics of a single-molecule magnet. This work aligns with ongoing efforts to develop methods for simulating time-resolved observables and required close collaboration between experimental researchers and large-scale research facilities. This work is being extended to further systems.

The Oxford team (Kirrander) published an article in *Nature Communications* examining the ultrafast photodissociation dynamics of the molecule morpholine. The combined experimental and theoretical study achieved extremely good time-resolution which made possible a very exacting comparison between simulations and experiment, revealing how distinct reaction channels contribute to the overall experimental observable. This work is now followed up by further simulation work to examine the role that the excitation energy plays in determining the branching ratio between the available reaction channels.

The UCL team (Worth) has been working on a number of systems. These include Criegee intermediates and glyoxylic acid, key molecules in atmospheric chemistry. The challenge here is the description of the dissociation channels that are hard for direct dynamics approaches due to the problems electronic structure methods have in describing bond breaking. A new direction in which the database at the heart of DD-vMCG calculations is initially populated with data for key geometries rather than just using data from the simulations is being trialled to improve the description of the asymptotic regions.

As described in detail in the previous report, the COSMOS Team co-led the prediction challenge on the photochemistry of cyclobutanone. Curchod and Worth co-organized a CECAM workshop in April 2025 to discuss the outcome of this challenge and are preparing a perspective article summarizing the outcome of this community exercise.

## **2.4 Workpackage 3. Simulating Quantum Technologies. Lead: DS.**

Leeds group has recently made a progress in applying Coherent States ideas towards the realm of electron dynamics. They published a communication in *The journal of Chemical Physics* describing a new concept of Particle Number Conserving Fermionic Coherent States for description of electronic wave functions showing how the most accurate Full Configuration Interaction wave function can be reproduced with a small number of PNFCSSs. This result may lead to a new direction in electronic structure theory.

The Leeds group has also made progress with using the methods developed in computational chemistry to model the dynamics of coupled qubits. In particular, it was demonstrated how  $SU(2)$  coherent states can serve as efficient basis set which follow short time dynamics.

Adam Kirrander and Dmitry Shalashilin hosted Professor Sebastian Fernandez-Alberti, one of the lead developers of quantum molecular dynamics software package NEXMD, during two months (Sep-Oct 2025) to discuss simulations in multichromophoric systems and large light harvesting systems, with an emphasis on suitable electronic structure methods and the theoretical treatment, potential experimental detection, and the physical role of large-scale molecular coherences.

## **3 Workshops and Training Activities**

### **3.1 Cohort Building and EDI. Lead: TJP.**

The cohort of PDRAs and PhD students participating in the project is listed in Sec. 8). Over the past year, Daniel Hollas (Bristol) has led the cohort representation and attended the Management Committee on behalf of the early career researchers (ECRs). From October, Julien Eng will take over this role. Julien and Daniel will work together during the handover to ensure continuity and to maintain the positive progress that has been made in building an engaged and supportive ECR community.

Several activities have taken place to develop the ECR cohort, provide skills training, and strengthen collaboration across the network. The Quantics Hackathon, held at Warwick on 16–17 June 2025, was attended exclusively by ECRs and provided an opportunity to collaborate on research problems in a supportive environment. The event helped promote peer learning and reinforced the value of the cross-site ECR network.

An ECR Career Development Meeting was also organised, featuring eight speakers from a range of academic backgrounds. This event highlighted different career pathways around academia, and included practical sessions on career planning. In addition, a professionally delivered presentation skills workshop was held to help ECRs improve clarity, delivery and confidence in presenting research. Feedback from participants was very positive and noted the usefulness of the training for upcoming conference and seminar presentations.

Looking ahead, several further initiatives are in development. A new ECR seminar series will be launched, in which Julien will invite ECRs to present their work at the different institutions. Those who volunteer will be supported in giving informal seminars within partner institutions, helping to raise visibility and build research links.

We are also preparing a short survey to assess how well supported ECRs currently feel, and to identify any further training or cohort support needs. To encourage regular informal interaction, we will trial

periodic online “coffee break” catch-ups. These will be optional and low-pressure, recognising that they may evolve naturally depending on engagement.

Finally, a Christmas get-together will be held, combining short talks with an informal social event, and plans are beginning for a second Hackathon, likely to be held in early next year.

### **3.2 Workshops Held 2024-2025**

- Quantics Hackathon, Warwick, 16-17 June 2025 [Scott]
- ECR Training in Presentation Skills, UCL 30 Apr - 1 May 2025 [Tom]
- Joint COSMOS - UPDICE meeting, UCL, 4-5 Aug. 2025 [Graham]
- CECAM Workshop on the Prediction Challenge, EPFL, 8-10 Apr 2025 [Basile /Graham]
- Theoretical Chemistry Graduate Student Meeting, online, 4-5 September 2025 [Basile]
- COSMOS XFEL Theory/Experiment Meeting, Imperial, 1-2 July 2025. [Basile/ Tom/ Adam / Graham]
- COSMOS Meeting on Electronic Structure, Oxford, 8-9 Sept 2025. 85 participants [Adam]

### **3.3 Planned**

1. Faraday Discussions, 'Molecular excited states theory and experiment', Cambridge, 14-16 September 2026.
2. Spectroscopy and Dynamics Meeting, RSC Interest Group, Warwick, 7-9 January 2026.

## **4 Exchange visits between members of COSMOS, internally and with project partners**

1. Leon Ashley (Penfold Group) visited the Worth group 10-12 Feb. 2025 to discuss coding a new adiabatic DD-vMCG algorithm.
2. Santoro (Pisa) visited the Worth group 18-22 Nov. 2024 to discuss the progress of the project to use Quantum Force fields combined with the DD-vMCG method to include solvent in excited state dynamics.
3. Agostini (Paris) hosted Basile Curchod to discuss the use of OpenFMS for the simulation of polaronic photochemistry in simple organic molecules. This topic is the main project of a PhD student who started in September 2025 in the Agostini group and will contribute to the OpenFMS code as part of COSMOS.
4. Fernandez-Alberti (Buenos Aires) visited the Kirrander and Shalashilin groups to discuss potential future links between the NEXMD code and QUANTICS, as well as scientific issues regarding large-scale coherences in molecular systems.
5. Leon Cigrang (Worth group) visited the Kirrander group 26-27 March 2025 to discuss clustering analysis of quantum molecular dynamics simulations.

6. Online meetings were organized between Claudia Magi, PhD student in the Agostini group (Paris), and members in the Curchod group to discuss implementations in OpenFMS as part of the COSMOS project.
7. Bonella (EPFL) organized discussions with members of the Curchod group at CECAM (Lausanne) as part of CECAM workshops to discuss implementations of novel framework to sample a Wigner distribution for molecular systems beyond the harmonic approximation.
8. Segarra-Martí and Curchod will co-organize a Faraday Discussion in September 2026 at Cambridge on excited molecular states and dynamics, theory and experiment.
9. Ingle (UCL) and Curchod organized regular meetings as part of a collaboration on the analysis of time-resolved photoelectron spectroscopy on a dual-emissive molecule (WP2).

## 5 Presentations at International Meetings and University Symposia

Worth has presented work related to COSMOS at:

1. Cecam Workshop: Future Directions in Non-adiabatic Dynamics: Towards Complex Systems and Long Time Scales, Zaragoza, Spain, Sep. 2-5 2025.
2. 29th Dynamics of Molecular Collisions, Snowbird, Utah, Jul. 6-11 2025.
3. 26th International Conference on the Jahn-Teller Effect, On-line, May 5-9 2025.

Penfold has presented work related to COSMOS at:

1. Satellite on Ultrafast Structural Dynamics, DESY User Meeting, Hamburg, Jan. 2025
2. Physical Chemistry Seminar, University of Mainz, Mainz, June 2025
3. Workshop Bringing together Theory and Large Scale Facilities, Leuven, Belgium, July 2025.
4. Theory for X-FELs, European X-FEL, Hamburg, Oct. 2025

Curchod has presented work related to COSMOS at:

1. CECAM Workshop 'Back to the future: Molecular simulation 40 years after Varenna', Rome, Italy, September 26 2025
2. EuXFEL Science Seminar, Hamburg, Germany, September 16 2025
3. 'COSMOS Electronic Structure Theory for Dynamics', Oxford, UK, September 4 2025.
4. Theoretical Photodynamics Workshop, Nantes, France, August 27 2025.
5. Workshop on Quantum Dynamics in Complex Systems, Telluride, Telluride, USA, July 7 2025.
6. Chemistry Lecture, Torun, Poland, May 16 2025.
7. ACS Spring Meeting, San Diego, USA, March 23 2025.
8. Physical Chemistry Seminar, USC, Los Angeles, USA, March 19 2025.
9. Lord Porter Lab Seminar, Sheffield (online), UK, February 24 2025.
10. Chemistry Seminar, Edinburgh, UK, December 18 2024.
11. CECAM workshop on material excited states, Lausanne, Switzerland, November 5 2024.
12. CECAM Webinar Series, virtual, October 17 2024.

Shalashilin and his group have presented work related to COSMOS at:

1. International Chemical Congress of Pacific Basin Societies 2025, Honolulu, Hawaii, USA, December 15-20, 2025.
2. 'COSMOS Electronic Structure Theory for Dynamics', Oxford, UK, September 4 2025.
3. Bohm in Brazil workshop, Sao-Paulo, Brazil, July 15-19 025
4. Quantemol Workshop. London, UK, April 2025.
5. CECAM workshop to discuss the results of the prediction challenge on the photochemistry of cyclobutanone, Lausanne, Switzerland, April 2025.

Habershon has presented work related to COSMOS at:

1. *Physics-informed program synthesis for quantum chemistry*, Telluride Science Research Centre Workshop on Quantum Dynamics in Complex Systems, Telluride, CO, USA, July 2025.
2. ca. 8 invited seminars at UK-based universities as part of a Royal Society of Chemistry lecture tour associated with Bourke-Liversidge award.

Kirrander has presented work related to COSMOS at:

1. SAGAMORE 2024, Delhi, India, 10-15 November 2024 (Invited presentation, given by postdoctoral research fellow Dr A. Moreno-Carrascosa).
2. EEC Symposium, Edinburgh, UK, 5 September 2025.
3. 2025 SSRL/LCLS User's Meeting, 21-26 September 2025 (Invited presentation, given by postdoctoral research fellow Dr M. Simmermacher).

## 6 Outreach Activities

1. Worth taught at the MCTDH Summer School, Heidelberg, Germany, Jul. 28 - Aug 1 2025.
2. Curchod taught at the CECAM School 'Quantum and Mixed Quantum Classical Dynamics in photochemistry', Zaragoza, Spain, March 31 - April 4 2025.
3. Penfold taught Introduction to Quantum Phenomena at Partners Summer School, Newcastle University July 2025.
3. Penfold hosted a RSC Summer Student studying quantum dynamics on complex systems.
4. Kirrander co-authored a community perspective paper on quantum information science in chemistry research, with a particular focus on quantum dynamics and ultrafast measurements [*J. Phys. Chem. Lett.*, **16**, 1376 (2025)], based on a NSF-EPSCRC workshop he co-organised in 2024.
5. Our art-science collaborator, artist Rupert Johnstone, trialled an interactive workshop in the Kirrander group, which will be rolled out as an ERC event during 2026. The collaboration has also resulted in the first physical objects inspired by the themes and topics of the COSMOS project.
6. Kirrander hosted an EPSCRC Summer Student studying quantum dynamics and ML methods.
7. Worth hosted a UCL Summer Student to study atmospheric chemistry using quantum dynamics.

## 7 Publications

1. Decoupling structural molecular dynamics from excited state lifetimes using few-femtosecond ultraviolet resonant dispersive waves, S. L. Jackson, A. W. Prentice, L. Bertram, L. Hutton, N. Kotsina, C. Brahms, C. Sparling, J. C. Travers, A. Kirrander, M. J. Paterson and D. Townsend, *Nat. Commun.*, 2025, 16, 9986  
<https://cosmosproject.co.uk/publications/jac25decoupling>
2. A new form of particle number conserving fermionic coherent states for electronic structure theory and electron dynamics, D. V. Shalashilin, D. V. Makhov, *J. Chem. Phys.* 2025, 163, 131102  
<https://cosmosproject.co.uk/publications/sha25anew>
3. The Singlet–Triplet Gap of Pyruvic Acid, E. M. Burrow, J. Carmona-García, C. J. Clarke, B. F. E. Curchod and J. R. R. Verlet, *J. Am. Chem. Soc.* 2025, 147, 41, 36987–36991  
<https://cosmosproject.co.uk/publications/bur25singlet>
4. Visualizing the Three-Dimensional Arrangement of Hydrogen Atoms in Organic Molecules by Coulomb Explosion Imaging. A. E. Green, K. Chen, S. Bhattacharyya, F. Allum, S. Usenko, M. N. R. Ashfold, T. M. Baumann, K. D. Borne, M. Brouard, M. Burt, B. F. E. Curchod, B. Erk, R. J. G. Forbes, L. M. Ibele, R. A. Ingle, H. V. Sa Lam, X. Li, K. Lin, T. Mazza, J. W. McManus, M. Meyer, T. Mullins, J. P. Figueira Nunes, D. E. Rivas, A. Roerig, A. Rouzée, P. Schmidt, J. Searles, B. Senfftleben, H. Stapelfeldt, R. M. P. Tanyag, F. Trinter, A. S. Venkatachalam, E. Wang, E. M. Warne, P. M. Weber, T. J. A. Wolf, T. Jahnke, A. Rudenko, R. Boll and D. Rolles, *J. Am. Chem. Soc.* 2025, 147, 41, 37133–37143  
<https://cosmosproject.co.uk/publications/gre25visualizing>
5. Benchmarking Electronic-Structure Methods for the Description of Dark Transitions in Carbonyls at and Beyond the Franck-Condon Point, J. Bone, J. Carmona-García, D. Hollas, and B. F. E. Curchod, *J. Phys. Chem. A*, 2025, 129, 9355-9367  
<https://cosmosproject.co.uk/publications/>
6. Perspective: Vibronic Coupling Potentials for Trajectory-Based Excited-State Dynamics, S. Gómez, P. Vindel-Zandbergen, D. Farkhutdinova, and L. González, *J. Chem. Theory Comput.* 2025, 21, 8634-8649  
<https://cosmosproject.co.uk/publications/gom25perspective>
7. Machine learning for nonadiabatic molecular dynamics: best practices and recent progress, C. Müller, Š. Sršeň, B. Bachmair, R. Crespo-Otero, J. Li, S. Mausenberger, M. Pinheiro, Jr, G. Worth, S. A. Lopez and J. Westermayr, *Chem. Sci.*, 2025, 16, 17542-17567  
<https://cosmosproject.co.uk/publications/mul25machine>
8. Is there anybody out there? Ultrafast Rydberg–valence interactions in the photodissociation of trimethylamine. D. J. Hughes, A. W. Prentice, L. Bertram, R. T. Chapman, L. Craciunescu, D. A. Horke, P. Krüger, M. A. Parkes, H. J. Thompson, E. Springate, J. O. F. Thompson, Y. Zhang, A. Kirrander, M. J. Paterson, and R. S. Minns. *J. Chem. Phys.*, 2025, 163, 074306  
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<https://cosmosproject.co.uk/publications/mer25triplets>
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<https://cosmosproject.co.uk/publications/san25tstrongfield>
13. Ultrafast ring-opening dynamics of 1,2-dithiane following ultraviolet absorption, P. A. Robertson, J. Merrick, D. Heathcote, M. S. Robinson, A. Butler, Y. Biddick, J. F. P. Nunes, C. Rankine, Z. Liu, S. F. Arrowsmith, J. O. F. Thompson, M. N. Murty, R. Chapman, E. Springate, E. A. Anderson, A. Kirrander and C. Vallance, *Chem. Phys. Lett.*, 2025, 871, 142095  
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## 8 Early Career Researchers on the Project

Dates	Name	Institution	Status	Employed on grant?
Oct. 2023 - Now	Eryn Spinlove	UCL	Programme Manager	Y
Jan. 2024 - Now	Sar bani Patra	UCL	PDRA	Y
Oct. 2023 - Now	Leon Cigrang	UCL	PhD	N
Oct. 2023 - Now	Jaymee Coonjobeeharry	UCL	PhD	N
Oct. 2024 - Now	Swagato Saha	UCL	PhD	N
Jul. 2024 - Now	Daniel Hollas	Bristol	PDRA	Y
Jun. 2024 - Now	Vera Brieskorn	Bristol	PhD	N
Jul. 2024 - Jul. 2025	Yorick Lassmann	Bristol	PhD	N
Jan. 2024 - Now	Julien Eng	Newcastle	PDRA	Y
Apr. 2024 - Now	Thomas Pope	Newcastle	PDRA	N
Oct 2023 - Now	Clelia Middleton	Newcastle	PhD	N
Oct 2024 - Now	Leon Ashley	Newcastle	PhD	N
Oct 2024 - Now	Lidice Cruz-Rodriguez	Warwick	PDRA	Y
Sep. 2025 - Now	Joe Gilkes	Warwick	PDRA	Y
Oct 2023 - Now	Zahra Bhatti	Warwick	PhD	N
Oct. 2025 - Now	Adam O'Hare	Warwick	PhD	N
Oct 2023 - Now	Dmitry Makhov	Leeds	PDRA	Y
Oct 2024 - Now	Michal Horansky	Leeds	PhD	N
Oct 2025 - Now	Ismaele Recca	Leeds	PhD	N
Oct 2023 - Now	Andrés Moreno Carrascosa	Oxford	PDRA	N
Oct 2023 - Now	Lewis Hutton	Oxford	PDRA	N
Oct 2023 - Now	Jakub Kara	Oxford	PhD	N
Oct 2023 - Now	James Merrick	Oxford	PhD	N

## 9 Members of the Project

The project has a group of international partners and associated researchers, listed below. Those marked with an asterisk have joined in the last year.

1. Federica Agostini, University Paris-Saclay
2. Mikhail Ivanov, Max-Born-Institute Berlin
3. Peter Weber, Brown University
4. Jakob Andreasson, ELI Beamlines
5. Matthias Kling, SLAC National Accelerator Laboratory
6. Eli Zysman-Colman, University of St. Andrews
7. Javier Segarra-Martí, University of València
8. Sergei Tretiak, Los Alamos National Lab

9. Hans Jakob Wörner, ETH Zürich
10. Nada Došlić, Ruđer Bošković Institute
11. Sandra Gómez, Universidad de Salamanca
12. Morgane Vacher, Nantes Université
13. Julia Weinstein, University of Sheffield
14. Olof Johansson, University of Edinburgh
15. Terry Frankcombe, UNSW Canberra
16. Shirin Faraji, Heinrich Heine University Düsseldorf / Rijksuniversiteit Groningen
17. Josh Vura-Weis, University of Illinois Urbana-Champaign
18. John Marangos, Imperial College London
19. Fabrizio Santoro, iCCOM Pisa
20. Sara Bonella, EPFL CECAM
21. Martin Centurion, University of Nebraska-Lincoln
22. Kenneth Lopata, Louisiana State University
23. Michael Minitti, SLAC (MeV-UED)
24. Daniel Rolles, Kansas State University
25. Cristina Sanz-Sanz, Universidad Autonoma de Madrid
26. Benjamin Lasorne, ICGM Montpellier
27. Albert Stolow, University of Ottawa
28. Michael Schuurman, University of Ottawa
29. Artur Izmaylov, University of Toronto
30. Oriol Vendrell, University of Heidelberg
31. Daniel Pelaez-Ruiz, ISMO Université Paris-Saclay
32. Irene Burghardt, Goethe University Frankfurt
33. Helen Fielding, University College London
34. Rebecca Ingle, University College London
35. Vas Stavros, University of Birmingham
- 36.\* Frank Grossmann, Technische Universität, Dresden
- 37.\* Rachel Crespo-Otero, University College London

38.\* Nanna Holmgaard-List, Birmingham University / KU Stockholm

Explicit work with the partners has been carried out as follows.

1. Worth has been working with Pelaez-Ruiz (Paris Sud) and Gómez (Madrid) on machine learning potential surfaces.
2. Curchod has been working with Agostini (Paris Sud) on developments with Multiple Spawning.
3. Worth has been working with Santoro (Pisa) on further developments using quantum force fields for excited-state dynamics.
4. Habershon has been working with Stavros (Birmingham) on integrated simulation/experimental studies of excited-states in maleimide fluorescent probes (manuscript in preparation).

## **10 Management Group Meetings**

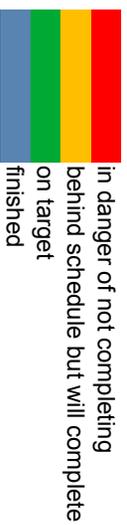
Meetings of the PIs on the project and Programme Manager have been held monthly. Discussions have been held on progress and future work, along with organisational details of meetings and ECR employment. Minutes of these meetings are available on request.

## **11 Appendix: Progress of Milestones**

In the following pages, the milestones for the 4 workpackages are presented, colour-coded to show progress.

## CA: Unified Code for Quantum Dynamics

Health	Milestone	Who	Due date	Status 10/25
	DCA.1	Whole Team	10/24	Zagreb TSH integrated Exact Factorisation integrated AIMS integration ongoing
	DCA.2a	EPCC, GW	6/26	Gitlab repository set up Quantics Control Group set up
	DCA2.b	ES, GW	6/25	SQLite DB format finalised Format of output files for external use still to be decided
	DCA.3	ES	10/24	Discourse Forum Active Web-site written: to be deployed soon
To start 11/25	DCA.4	EPCC, GW, BC	10/27	Tests have been run to identify bottlenecks.
	DCA.5	Whole Team	6/26	New QC interface module complete
	DCA.6	ES, GW	10/25	Prototype Quantics GUI written
	DCA.7	Whole Team	6/27	Ongoing.



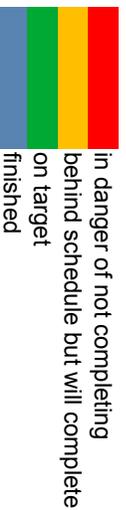
## WP1: New Methods for Quantum Dynamics

Health	Milestone	Who	Due date	Status 10/25
Yellow	D1.1a Sampling Strategies	BFEC, DS	3/25	New strategies implemented in AIMS.
Green	To start 10/26 D1.1b Numerical Stability	BFEC, SH, DS, GW	9/28	DD-VMCG with light pulses implemented.
Green	D1.2 Couple QD to external perturbations	AK, TJP, GW	9/26	New NN fitting from DD-VMCG databases. GPR fitting added to VCHAM – not yet finished
Green	D1.3a ML/AI potentials	SH, TJP, GW	9/26	
Green	D1.3b New AI/ML-driven QD for long time scales	SH / TJP	9/29	
Green	To start 10/26 D1.4 New solid-state QD schemes	TJP	9/29	

■ in danger of not completing  
■ behind schedule but will complete  
■ on target  
■ finished

## WP2: Quantum Dynamics in Chemistry

Health	Milestone	Who	Due date	Status 10/25
	D2.1 Implementation of methodologies simulating a range of time and energy resolved observables from QD simulations. Validation of theoretical methods with experimental observables:	BFEC, SH, AK, TJP, GW	10/26	PDA (pump pulse), TRXRS/TRUED code (IAM), TRXAS, Quantum thermostat
	D2.2 photodamage and photoprotection; photoredox catalysis; fluorophores oligorisation atmospheric chemistry, sunscreens / crop additives. light emitting / converting materials	SH, BFEC, TJP, GW BFEC, TJP	12/25 9/29	Theory/experiment study of photoredox DDQ completed (BFEC, TJP). Studies on fluorophores underway (GW) Theory/experiment study of atmospheric photochemistry underway
To start 1/27 To start 10/28 To start 11/25	D2.2e,f D2.2g,h	GAW, BFEC BFEC	9/29 6/29	Preliminary work initiated in the group Oct-28 of TJP (LVC models of TADF). AIMS and initial conditions lecture (BFEC) at Workshop on Theoretical Quantics workshop (GW) at the MCTDH Summer School (Heidelberg Sept. 2025)
	D2.3 Design models for photoredox catalysis and TADF	BFEC, TJP		
	D2.4 Training			



### W/P3: Simulating Quantum Technologies

Health	Milestone	Who	Due date	Status 10/25
D3.1a	electron dynamics in a strong field	AK, DS, GW	9/26	
To start 10/26	electron attosecond dynamics, scattering and imaging			
D3.1b	Spin CS for coupled Qubits	AK, DS	9/29	
D3.2a	Simulations of coupled Qubits	BFEC, DS	9/26	
D3.2b	Molecular Qubits, Cr Complexes	BFEC, DS	9/26	
To start 1/27	Electronic structure calculations based on CS algorithms	BFEC	3/29	
D3.3	New approaches for simulating bosonic systems	AK, DS	9/29	
D3.4		DS	9/29	
D3.5	Coherent State modules for Quantics	BC, AK, DS, GW	9/29	Implementation as part of AIMMS package underway

█ in danger of not completing  
█ behind schedule but will complete  
█ on target  
█ finished