UNIVERSITY OF CAMBRIDGE

Yusuf Hamied Department of Chemistry

Postgraduate Virtual Open Day 2024

"Welcome to Cambridge, and welcome to the Yusuf Hamied Department of Chemistry postgraduate open day.

We pride ourselves on having world-class research activity that covers a very broad range of topics, and I hope that you will find something here which captures your imagination and makes you want to join us.

In the Department you will be working alongside top-rate researchers, so you can expect an exciting and challenging experience. We provide a supportive environment in which everyone can flourish scientifically and develop personally.

We welcome applications from ambitious and dedicated students from around the world."

Professor James Keeler, Head of Department

Postgraduate Virtual Open Day Schedule

Yusuf Hamied Department of Chemistry, University of Cambridge

Thursday 7th November 2024

11:00 – 11:20	**Postgraduate Team Presentation**
11:20 – 11:45	**Q&A**

Acknowledgements

Organisers *Dr David Morgan, Olivia Hamlet*
Photography *Nathan Pitt and Michael Webb*
Design *Richard Shaw*

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The Yusuf Hamied Department of Chemistry

University of Cambridge

Our Department ranks as the top Chemistry department in the UK and among the top five in the world.

We have roughly 70 academic staff, 200 postdocs, and 300 postgraduate students. We receive at least 500 applications a year from prospective postgraduate students, admitting around 80 in total. We offer the following postgraduate degrees:"

MPhil in Chemistry *(by research)*
PhD in Chemistry

The Department expanded in 2018 with the new £23M Chemistry of Health Centre. This is a state of the art hub for the Centre for Protein Misfolding Diseases and the Molecular Production and Characterisation Centre.

We are actively engaged in improving the under-representation of women in science and we are proud to have received the Athena SWAN Silver Award. Women scientists currently make up 43% of our postgraduates and 35% of our postdocs.

Our entire postgraduate student body is extremely well supported by a team of dedicated staff, a pastoral tutor group and very well established student and academic mentoring systems.

Admissions Contact
admissions@ch.cam.ac.uk

How To Apply

The Route into Cambridge

Successful applications come from people who have researched what they want to study and with whom. That is our experience. While success in the process cannot be guaranteed, a well-researched and thoroughly written application is the expectation. We encourage you to correspond directly with potential supervisors in advance of submitting your application.

To be considered for Departmental funding (as well as the University scholarship competitions) your application must be submitted by 3rd December 2024. Submit your application using the University Postgraduate Admissions online Applicant Portal. Checking documents requirements early on is advised to avoid delays or automatic rejection and submitting early is desirable.

The Department has minimum entry requirements which are higher than some other departments across the University:

MPhil 2.1 Honours degree
PhD 2.1 MSci or MChem

Please check here for international equivalencies and if you are still unsure, contact the Chemistry Postgraduate Admissions Team.

University Postgraduate Admissions
For application submissions, scholarship searching and more, please click here.

Chemistry Postgraduate Admissions
For details on how to apply, application guidance, funding options and links, please click here.

Postgraduate Education

Our Researcher Development Programme

The Department of Chemistry is committed to providing an excellent postgraduate experience for everyone through wide-ranging training activities and social events.

Our postgraduate students attend research level lectures and workshops throughout their time here. They also get involved in our researcher development programme including transferable skills and employability workshops. We offer in-house careers sessions as well as promote relations with the University Careers Service.

There are a lot of opportunities to supervise undergraduates and demonstrate in the laboratories, both of which offer a means to learn a new skill, as well as being a mechanism to generate a modest additional income.

The Cambridge undergraduate education system uses an intensive tutorial system (supervisions) led by PhD students, postdocs and academics. The best way to get involved is through the Colleges.

Demonstrating in undergraduate labs is seen as a core part of Postgraduate Education. This brings with it the responsibility of guiding practical sessions, demonstrating lab techniques and marking experimental reports.

Postgraduate Education Contact
postgraduate.education@ch.cam.ac.uk

Materials Chemistry

Our Dark & Light-Emitting Materials

The technological devices we depend on, from aeroplanes to mobile phones, rely upon ever-increasing structural complexity for their function. Designing complex materials for these devices through the art of chemical synthesis brings challenges and opportunities.

Members of the Materials RIG invent new materials in view of potential applications. Modern materials chemistry is a wide ranging topic and includes surfaces, interfaces, polymers, nanoparticles and nanoporous materials, self assembly, and biomaterials, with applications relevant to oil recovery and separation, catalysis, photovoltaics, fuel cells and batteries, crystallisation and pharmaceutical formulation, gas sorption, energy, functional materials, biocompatible materials, computer memory, and sensors.

If you are keen to work on a project in one of our groups, contact the group leader directly and discuss your application with them in advance of submitting your application to the University.

The Materials Chemistry research groups accepting postgraduate students (PhD and MPhil) for entry in October 2025 are:

Prof. Hugo Bronstein

Prof. Melinda Duer

Prof. Alex Forse

Prof. Clare Grey FRS

Dr Svetlana Menkin

Prof. Jonathan Nitschke

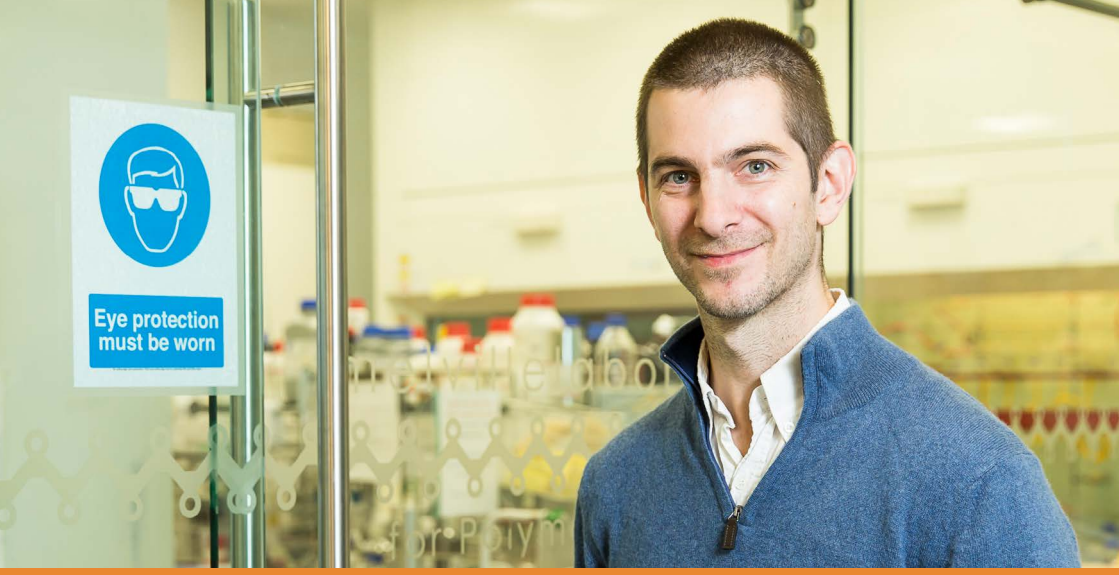
Prof. Erwin Reisner

Prof. Oren Scherman

Prof. Andrew Wheatley

Prof. Dominic Wright

Dr Jenny Zhang



Professor Hugo Bronstein | click here for video

Organic Materials for Energy Applications

Research in our group is centred on the organic synthesis of conjugated polymers and molecules for a range next generation plastic electronic technologies.

Key challenges are the development of flexible solar panels and light emitting diodes which are flexible, efficient and sustainable. We also research many other aspects of functional organic materials such as bio-electronics, flexible lasers and field-effect transistors.

We work closely with physicists and materials scientists to understand the underlying photophysical processes in our materials and test them as a new generation of plastic electronic devices.

Relevant Papers

Synthesis of model heterojunction interfaces reveals molecular-configuration-dependent photoinduced charge transfer. *Nature Chemistry*, **2024**, 16, 1453–1461.

Suppression of Dexter transfer by covalent encapsulation for efficient matrix-free narrowband deep blue hyperfluorescent OLEDs. *Nature Materials*, **2024**, 23, 519–526.

Exploiting Excited-State Aromaticity To Design Highly Stable Singlet Fission Materials. *J. Am. Chem. Soc.*, **2019**, 141, 13867–13876.

Highly Luminescent Encapsulated Narrow Bandgap Polymers Based on Diketopyrrolopyrrole. *J. Am. Chem. Soc.*, **2018**, 140, 1622–1626.

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Professor Melinda Duer | click here for video

Understanding How Materials Direct Cell Behaviour

We use solid-state NMR, electron microscopy and a range of optical imaging techniques to understand the key molecular structural and dynamics aspects of the extracellular matrix and biomaterials that drive cell behaviour.

The extracellular matrix (ECM) is a complex 3D architecture of proteins and sugar polymers. It forms the bulk of our structural tissues and provides them with their particular mechanical properties but more intriguingly, at the molecular level, it provides the communication system between the cells in the tissue and the signals that drives the individual behaviour of cells. The ECM is particularly important in degenerative diseases, such as osteoporosis, osteoarthritis, diabetes mellitus and neurodegenerative diseases, and in cancer, where. degradation of the ECM directs dysfunctional cell behaviour that progresses the disease. Our aim is to generate insight that leads to chemistry-based approaches to repairing damaged or aberrant ECM structures to restore cell, and hence organ, function.

Relevant Papers

Glycation changes molecular organization and charge distribution in type I collagen fibrils. Sneha Bansode, Uliana Bashtanova, Rui Li, Jonathan Clark, Karin H. Müller, Anna Puszkarska, Ieva Goldberga, Holly H. Chetwood, David G. Reid, Lucy J. Colwell, Jeremy N . Skepper, Catherine M. Shanahan, Georg Schitter, Patrick Mesquida, Melinda J. Duer*, *Scientific Reports*, 10 **(2020)** 3397-3410.

Collagen Structure–Function Relationships from Solid-State NMR Spectroscopy. Ieva Goldberga, Rui Li, and Melinda J. Duer*, *Acc. Chem. Res*. 51 **(2018)** 1621-1629.

Citrate bridges between mineral platelets in bone. E. Davies, K.H. Muller, W.C. Wong, C. J. Pickard, D.G. Reid, J.N. Skepper, M.J. Duer*, *Proc. Nat. Acad. Sci. USA* 111 **(2014)** E1354–E1363

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Professor Alex Forse | click here for video

Materials for Climate Change Mitigation

Our ultimate goal in the Forse Group is to design materials that can reduce greenhouse gas emissions and help tackle the climate crisis. Limiting global warming to 1.5 °C requires the rapid development and deployment of a range of greenhouse gas mitigation technologies.

We are exploring new materials for carbon dioxide capture and electrochemical energy storage, both of which can help mitigate greenhouse gas emission. For example, we are developing new batteries that can capture carbon dioxide pollution when charged. We are also developing improved fast charging supercapacitor energy storage devices.

We specialise in the application of nuclear magnetic resonance (NMR) spectroscopy techniques that are complemented by electrochemistry, synthetic chemistry and computational chemistry.

Relevant Papers

Capturing Carbon Dioxide from Air with Charged Sorbents, *Nature*, **2024**, 630, 654

Structural Disorder Determines Capacitance in Nanoporous Carbons, *Science*, **2024**, 384 (6693), 321

Enhancing Electrochemical CO2 Capture with Supercapacitors, *Nature Comm.* **2024**, 15, 7851

Revealing Ion Adsorption and Charging Mechanisms in Layered Metal-Organic Framework Supercapacitors with Solid-State Nuclear Magnetic Resonance, *J. Am. Chem. Soc.*, **2024**, 146, 33, 23171

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Professor Dame Clare P. Grey FRS | click here for video

Structure and Dynamics in Batteries and Supercapacitors

We use a wide range of techniques, including solid state NMR spectroscopy and diffraction, to investigate local structure and dynamics and the role that this plays in controlling the physical properties of technologically important, but disordered materials. A particular focus of the group is on understanding how the materials that are found in rechargeable batteries – such as those found in laptops, mobile phones and electric vehicles - function. For example, if we can determine how Li-ions move in and out of the battery electrode materials, as the batteries are cycled, then we could design materials that could sustain even faster cycling or may last longer. Battery materials operate outside their thermodynamic stability windows and will react over time to form more stable structures, resulting in battery degradation. Our work focusses on understanding and mitigating these processes – with a particular emphasis on developing new characterization methods to follow these processes often in real time. With magnetic resonance methods we can watch, for example, Li plating and help provide insight into why this process (which can lead to serious safety incidents) occurs.

Relevant Papers

Niobium tungsten oxides for high-rate lithium-ion energy storage, *Nature*, **2018**, *559*, 556.
Materials' methods: NMR in battery research, Chem. Mater., **2017**, 29, 213-242.

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Dr Svetlana Menkin | click here for video

Fundamental studies of Electrified Interfaces and Electrodeposition enable Sustainable Batteries.

Our research aims to provide a fundamental understanding of localised interface activity and use the insights to enable sustainable, reliable, and affordable energy storage solutions for climate change mitigation. We look at metal electrodeposition mechanisms by investigating how a charge is transported across interfaces, one of the remaining fundamental questions in Electrochemistry. Using scanning electrochemical microscopy to focus on localised electrochemical reactions on the surface and electrochemical impedance spectroscopy to track charge passage routes through the solid-liquid interface, we gain new insights into how interface structure and dynamics drive bulk activity.

We explore new strategies for plating the most promising, albeit challenging, multivalent metals (e.g., calcium, zinc, and aluminium) that are still considered (almost) impossible to plate. At the same time, we are investigating lithium and sodium metal plating and corrosion using an alternative bottom-up methodology to realise safer and more energy-dense anode-free batteries.

Relevant Papers

[1] S. Menkin, J. B. Fritzke, R. Larner ,C. de Leeuw, Y. Choi, A. B. Gunnarsdóttir and C. P. Grey, *Faraday Discuss.*, **2023**,

[2] D. M. C. Ould, S. Menkin, H. E. Smith, V. Riesgo-Gonzalez, E. Jónsson, C. A. O'Keefe, F. Coowar, J. Barker, A. D. Bond, C. P. Grey, D. S. Wright, Angew. Chem. Int. Ed., 2022, 61, e202202133; *Angew. Chem.*, **2022**, 134, e202202133.

[3] Svetlana Menkin, Christopher A. O'Keefe, Anna B. Gunnarsdóttir, Sunita Dey, Federico M. Pesci, Zonghao Shen, Ainara Aguadero, and Clare P. Grey, *The Journal of Physical Chemistry C*, **2021**, 125 (30), 16719.

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Professor Jonathan Nitschke | click here for video

Strange Cages for Chemical Beasts

Simple organic subcomponents can come together around metal-ion templates to produce intricate hollow capsules.[1] The Nitschke group explores the design and uses of some of these three-dimensional architectures, along with the use of the same construction principles to produce interlocked structures – catenanes[2] and knots[3] – and double-helical metallopolymers with useful optoelectronic properties.[4] Some of the structures that we have explored include a tetrahedral cage that encapsulates white phosphorus,[5] an antiaromatic-walled cage,[6] and a large capsule isomorphous to ferritin.[7] Current work targets the preparation of dodecahedral capsules that will be large enough to encapsulate proteins, along with flexible capsules woven together from macrocyclic strands.

Relevant Papers

[1] D. Zhang, T. K. Ronson, J. R. Nitschke, Acc. Chem. Res. 2018, 51, 2423-2436.

[2] C. S. Wood, T. K. Ronson, A. M. Belenguer, J. J. Holstein, J. R. Nitschke, Nature Chem. 2015, 7, 354-358.

[3] J. P. Carpenter, C. T. McTernan, J. L. Greenfield, R. Lavendomme, T. K. Ronson, J. R. Nitschke, Chem 2021, 7, 1534-1543.

[4] J. L. Greenfield, D. Di Nuzzo, E. W. Evans, S. P. Senanayak, S. Schott, J. T. Deacon, A. Peugeot, W. K. Myers, H. Sirringhaus, R. H. Friend, J. R. Nitschke, Adv. Mater. 2021, 33, 2100403.

[5] P. Mal, B. Breiner, K. Rissanen, J. R. Nitschke, Science 2009, 324, 1697-1699.

[6] M. Yamashina, Y. Tanaka, R. Lavendomme, T. K. Ronson, M. Pittelkow, J. R. Nitschke, Nature 2019, 574, 511-515.

[7] J. A. Davies, T. K. Ronson, J. R. Nitschke, Chem 2022, https://doi.org/10.1016/j.chempr.2022.1001.1003.

[8] J. L. Greenfield, F. J. Rizzuto, I. Goldberga, J. Nitschke, Angew. Chem., Int. Ed. 2017, 56, 7541-7545.

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Professor Erwin Reisner | click here for video

Solar-Driven Chemistry

My group is interested in chemical aspects of Energy and Sustainability, in particular the conversion of solar energy into renewable fuels and high-value organic chemicals.

Thus, electro- and photocatalysis are central to our work at the interface of synthetic chemistry, materials and nano-science, chemical biology and engineering.

A central theme is the study and mimicry of natural processes such as plant photosynthesis and enzymes relevant for light-driven chemical synthesis.

Relevant Papers

Floating perovskite-BiVO4 devices for scalable solar fuel production, *Nature*, **2022**, 608, 518.

Photoelectrochemical CO2-to-fuel conversion with simultaneous plastic reforming, *Nature Synthesis*, **2022**, 2, 182

Solar-driven liquid multi-carbon fuel production using a standalone perovskite–BiVO4 artificial leaf, *Nature Energy*, **2022**, 8, 629

Bacteria–photocatalyst sheet for sustainable carbon dioxide utilization, *Nature Catalysis*, **2022**, 5, 633

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Professor Oren A. Scherman | click here for video

Dynamic Supramolecular Materials

Research in the Scherman Group uses host-guest chemistry to design dynamic materials with tailored properties. We employ cucurbit[n]uril macrocycles to control molecular-level interactions and assembly at colloidal, polymeric and small molecule interfaces. Our expertise spans organic synthesis, materials design and testing. The materials we develop have significant potential in both the healthcare and energy sectors. In healthcare, we are advancing materials for early disease detection, long-term monitoring, and targeted drug delivery — all aimed at improving patient outcomes and treatment options. Our high-performance biomaterials, such as artificial cartilage, demonstrate exceptional compressibility and strength for real-world use. We also develop sustainable and adaptable materials, including supramolecular systems for energy and electron transfer, storage technologies and catalysis. We are also interested in soft bioelectronic materials for wearables, robotics and as autonomous power sources. Our interdisciplinary approach combines fundamental chemistry with materials science for practical applications. We collaborate closely with departments including physics, engineering and the clinical school alongside maintaining strong industry partnerships.

Relevant Papers

Highly stretchable dynamic hydrogels for soft multilayer electronics, *Sci. Adv.*, **2024**, 10, eadn5142

Associative pyridinium electrolytes for air-tolerant redox flow batteries, *Nature*, **2023**, 103, 949-955

Highly Compressible Glass-like Supramolecular Polymer Networks, *Nat. Mater.*, **2022**, 21, 103.

Mechanically matching the rheological properties of brain tissue for drug-delivery in human glioblastoma models, *Biomaterials*, **2021**, 276, 120919

Nanoparticle Surfactants for Kinetically Arrested Photoactive Assemblies to Track Light-induced Electron Transfer, *Nat. Nanotechnol.*, **2021**, 16, 1121

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Professor Andrew Wheatley | click here for video

Exploiting synergy in multiscale systems

We are interested in generating new functionality by the multiscale integration of different chemical motifs.

A track-record in organometallics enables us to combine enhanced chemical reactivity with nanocatalyst design. We seek to harness the potential of synergic activity in multimetallic nanomaterials by developing both compositional and morphological control during synthesis. Our focus is on independently varying these two characteristics to allow new efficiencies in applications like oxygen and CO2 reduction or photocatalytic pollution abatement. We employ molecular control to manipulate crystal faceting, particle growth, and intermetal electronic effects.

We are also hosting molecules and nanomaterials in composites that combine the properties of the dopant with those of a support matrix. The latter is typically a conformed metal-organic framework. New ways of constructing these monolithic systems allow the combination of excellent mechanical properties with porosity and may also introduce additional functionality, e.g. if the support has a nonlinear optical nature. Composites offer potential in catalyst recycling, fuel synthesis and storage, and upconversion.

Relevant Papers

Manipulating morphology and composition in colloidal heterometallic nanopods and nanodendrites, *Nanoscale*, **2023**, 15, 8814.

The future of fuel: metal-organic frameworks for high density gas storage, *J. Am. Chem. Soc.*, **2020**, 142, 8541.

A one-pot route to faceted FePt-Fe3O4 dumbbells: probing morphology-catalytic activity effects in O2 reduction catalysis, *Adv. Funct. Mater.*, **2020**, 2002633.

Sol-gel synthesis of robust metal-organic frameworks for nanoparticle encapsulation, *Adv. Funct. Mater.*, **2018**, 1705588.

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Professor Dominic Wright | click here for video

From Molecules to Materials

Making new inorganic molecules and materials is fundamentally important to future developments in energy storage and catalysis. Our group is interested in broad aspects of synthetic inorganic chemistry, spanning main group elements and transition metals. The focus is on the development of systematic synthetic methods in inorganic synthesis, which parallel the type of synthetic approaches used in organic chemistry. Using these approaches we are exploring new strategies to molecular and extended materials, with applications in pollution control, water splitting, new-generation batteries and sustainable catalysis involving non-transition metals.

Relevant Papers

Single-Source Bismuth (Transition Metal) Polyoxovanadate Precursors for the Scalable Synthesis of Doped BiVO4 Photoanodes, ***Adv. Mater.***, **2018**, *30*, 1804033.

Theory and Practice: Bulk Synthesis of C3B and its H2- and Li- Storage Capacity, ***Angew. Chem. Int. Ed.,*** **2015**, *54*, 5919.

Dipole-Induced Band-Gap Reduction in an Inorganic Cage, ***Angew. Chem. Int. Ed.***, **2014**, *53*, 1934.

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Dr Jenny Zhang | click here for video

Biological and Artificial Photosynthesis

We love working at the intersections of science and are currently blending together materials science, engineering, electrochemistry, biophysics and chemical biology to understand how to better exchange energy/electrons with living systems. One part of our group develops toolsets to probe deep into the fascinating light-driven redox chemistry that underlies natural photosynthesis. Another part aims to re-wire photosynthesis using electrodes, molecular and colloidal electron shuttles to enhance its efficiency or to extract bioelectricity. We are also getting more inventive with ways in which we can apply our toolsets for manipulating the bioenergetics of living systems – the sky is the limit to what we can use these for.

Relevant Papers

Photosynthesis re-wired on the pico-second timescale, *Nature*, **2023**, 615, 836

3D-printed hierarchical pillar array electrodes for high-performance semi-artificial photosynthesis, *Nature Materials*, **2022**, 21, 811

Advancing photosystem II photoelectrochemistry for semi-artificial photosynthesis, *Nat. Rev. Chem.*, **2020**, 4, 6

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Synthetic Chemistry

Delivering diverse and pioneering synthesis methods

The Department's Synthetic Chemistry research is focussed on developing innovative new methods to make and use molecules of function.

Our interests range from innovative catalytic strategies to the synthesis of small molecules and beyond, to supramolecular assemblies or the total synthesis of biologically important compounds and natural products.

Our research is diverse, pioneering and internationally leading. The dynamic environment created by our research groups, working at the cutting edge of the field, makes postgraduate research at Cambridge the best place for outstanding and motivated students.

If you are keen to work on a project in one of the Synthetic Chemistry groups, contact the group leader directly. Discuss your application with them in advance of submitting your formal application form to the University.

The Synthetic Chemistry research groups accepting postgraduate students (PhD and MPhil unless otherwise indicated) for entry in October 2025 are:

Dr Pawel Dydio

Prof. Matthew Gaunt (PhD only)

Prof. Jonathan Goodman

Prof. Chris Hunter

Prof. Robert Phipps (PhD only)

Prof. David Spring

Dr Ruth Webster

Dr Pawel Dydio | click here for video

Our research aims to enable the clean and efficient synthesis of chemicals and materials through the systems of cooperative catalytic reactions and the advancement of catalysis based on a detailed mechanistic understanding of these processes at the molecular level. Our program focuses on valuable chemical transformations, for which there are no satisfactory alternatives, or the existing methods remain cumbersome. Hence, although the research is primarily curiosity-driven, it may immediately lead to innovations of practical significance. We have three intertwined and complementary research lines (i) multicatalysis via embedding cooperative reactions into artificial metabolic-like systems, (ii) mechanistically driven discovery of new valuable catalytic transformations, and (iii) addressing the limitations of established important catalytic processes based on elucidating their mechanistic features.

Relevant papers

Dual-Catalytic Transition Metal Systems for Functionalization of Unreactive Sites of Molecules. *Nat. Catal.* **2019**, 2, 114.

Binuclear Pd(I)–Pd(I) Catalysis Assisted by Iodide Ligands for Selective Hydroformylation of Alkenes and Alkynes. *J. Am. Chem. Soc.* **2020**, 142, 18251.

Isoselective Hydroformylation of Propylene by Iodide-Assisted Palladium Catalysis. *Angew. Chem. Int. Ed.* **2022**, 61 (17), e202116406.

Transfer C–H Borylation of Alkenes under Rh(I) Catalysis: Insight into the Synthetic Capacity, Mechanism, and Selectivity Control. *Chem Catal.* **2022**, 2, 762.

Photoinduced Cu(II)-Mediated Decarboxylative Thianthrenation of Aryl and Heteroaryl Carboxylic Acids. *Angew. Chem. Int. Ed.* **2024**, e202410616.

A Merger of Relay Catalysis with Dynamic Kinetic Resolution Enables Enantioselective β-C(Sp 3)–H Arylation of Alcohols. *Angew. Chem. Int. Ed.* **2024**, e202408418.

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Professor Matthew Gaunt | click here for video

Synthetic Chemistry in the Gaunt Group

Research in our group is centred on organic synthesis and catalysis. We are inspired by the pursuit of new concepts in synthetic organic chemistry involving transition metal catalysis, enantioselective catalysis, protein and nucleic acid modification and bioorthogonal chemistry, total synthesis of natural products and pharmaceuticals and high throughput experimentation methods to accelerate discovery in synthesis. This diverse range of synthesis-driven research areas provides a stimulating and dynamic environment that is enabled by outstanding students and postdocs working at the frontiers of the field. We also collaborate with the pharmaceutical industry and other academic groups in Chemical Engineering, Computation, Machine Learning, Drug Discovery and Molecular Biology.

In the Gaunt Group we are committed to providing a welcoming and supportive space for all. We are a sociable group and actively work to create an environment where everyone is free to be themselves. All members are encouraged to contribute to our scientific community where the sharing of knowledge and development of ideas forms the foundations of the group.

Relevant Papers

A General Catalytic β-C–H Carbonylation of Aliphatic Amines to β-Lactams. ***Science***, **2016**, 354, 851.

Multicomponent synthesis of tertiary alkylamines by photocatalytic olefin-hydroaminoalkylation, ***Nature***, **2018**, 561, 522.

A Protein Functionalization Platform Based on Selective Reactions at Methionine Residues, ***Nature***, **2018**, 562, 568.

A general carbonyl alkylative amination for tertiary amine synthesis, ***Nature***, **2020**, 581, 415.

Selective Chemical Functionalization at N6-Methyladenosine Residues in DNA Enabled by Visible-Light-Mediated Photoredox Catalysis, ***J. Am. Chem. Soc.*** **2020**, 142, 51

Multicomponent alkene azido-arylation by anion-mediated dual catalysis, ***Nature***, **2021**, 598, 597

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Professor Jonathan Goodman | click here for video

Molecular Challenges

In order to make molecules effectively, we need to be able to understand reactivity and selectivity, get the maximum possible information from analytical data, be able to predict adverse effects, and handle chemical data effectively. We address all of these issues, using machine learning and computational methods to improve our knowledge of chemistry.

Projects in our group include the development of new reactions (what are the limits of the possible?), the automated analysis of analytical data (have we have made what we think we have made?) and the prediction of properties (will a new molecule be safe and stable for as long as we need it to be?) Underlying all of this we are developing ways to enable people to store and analyse molecular data more consistently in order to maximise the impact of research.

Relevant Papers

Leveraging Language Model Multitasking To Predict C–H Borylation Selectivity, *J. Chem. Inf. Model.* 2024, **64**, 4286-4297.

Reaction dynamics as the missing puzzle piece: the origin of selectivity in oxazaborolidinium ion-catalysed reactions, *Chemical Science*, 2023, **14**, 12355-12365.

The DP5 Probability, Quantification and Visualisation of Structural Uncertainty in Single Molecules, *Chemical Science*, 2022, **13**, 3507-3518.

InChI version 1.06: now more than 99.99% reliable, *J. Cheminformatics*, 2021, **13**, 40.

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Professor Chris Hunter

Organic Chemistry

Our research is based on the design and synthesis of organic molecules to learn fundamental rules that govern the complex relationship between chemical structure and functional properties. Current projects include synthetic oligomers that copy sequence information from parent to daughter strands using template-directed synthesis, synthetic signal transduction systems that transfer chemical information across lipid bilayer membranes, multivalent ligands for diagnosis and treatment of protein misfolding diseases, computational and physical organic studies of the role of solvation in solution phase equilibria. Projects may involve a range of different techniques and approaches including supramolecular chemistry, organic synthesis, physical organic chemistry, computational modelling, analytical chemistry and chemical biology. We also have active collaborations with the pharmaceutical and agrochemical industry and with academic research groups in other disciplines across Europe, providing opportunities to learn new skills in different environments.

Relevant Papers

Selective Duplex Formation in Mixed Sequence Libraries of Synthetic Polymers, *J Am Chem Soc* **2024**, 146, 9326.

An atomic surface site interaction point description of non-covalent interactions, *Chem Sci* **2024**, 15, 160.

Ligand Profiling as a Diagnostic Tool to Differentiate Patient-Derived α-Synuclein Polymorphs, *ACS Chem Neurosci* **2024**, 15, 2080.

Replication of Synthetic Recognition-encoded Oligomers by Ligation of Trimer Building Blocks, *Org Chem Front* **2023**, 10, 5950.

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Professor Robert Phipps | click here for video

Exploiting Non-covalent Interactions for Control in Catalysis

Our primary focus is on the design and development of new catalysts that employ non-covalent interactions (such as hydrogen bonds, ion pairs) to control various aspects of selectivity. These aspects include regioselectivity, site-selectivity and enantioselectivity, all of which are crucial elements that need to be carefully controlled for a useful synthetic process.

Non-covalent interactions are used extensively by enzymes in biological catalysis and also by supramolecular chemists to assemble fantastic macromolecular structures. Harnessing non-covalent interactions in the context of small molecule catalysts to advance the field of synthetic organic chemistry has fantastic potential and this is our group's main interest.

A range of projects encompass reactivity through transition metals as well as free radicals and we have a number of studentship collaborations with the pharmaceutical industry.

Relevant Papers

A Chiral Hydrogen Atom Abstraction Catalyst for the Enantioselective Epimerization of Meso Diols. *Science* **2024**, 386, 42.

Enantioselective Nitrene Transfer to Hydrocinnamyl Alcohols and Allylic Alcohols Enabled by Systematic Exploration of the Structure of Ion-Paired Rhodium Catalysts *J. Am. Chem. Soc*. **2024**, 146, 22629

sSPhos: A General Ligand for Enantioselective Arylative Phenol Dearomatization via Electrostatically-Directed Palladium Catalysis *J. Am. Chem. Soc.* **2023**, 145, 25553

"The Discovery and Development of the Enantioselective Minisci Reaction" *Acc. Chem. Res.* **2023**, 56, 2037

Strategies That Utilize Ion Pairing Interactions to Exert Selectivity Control in the Functionalization of C-H Bonds *J. Am. Chem. Soc.*, **2022**, 144. 18195

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Professor David Spring | click here for video

Chemistry at the interface with Biology and Medicine

Our research interests use organic synthesis to make molecules, which can be utilised to understand and exploit biological systems. Our current projects include improved designs for antibody-drug conjugates, next generation peptide therapeutics, synthetic methodology, and the discovery of new antibiotics. We collaborate with many chemical companies and academic groups around the world.

The scientific education of our group members in organic synthesis is given a high priority. All of our postgraduate students are encouraged also to learn new techniques relating to their projects with our industrial and academic collaborators.

Every effort is made so that group members achieve their career ambitions, usually jobs in academia or the chemical industries.

Relevant Papers

R. Walther, M. Park, N. Ashman, M. Welch, J. S. Carroll, D. R. Spring. Tuneable thiol exchange linkers for traceless drug release applications in prodrugs and ADCs. *Chem. Commun.* **2024**, 60, 7025-7028. https://doi.org/10.1039/D4CC01558D

T. Wharton, F. Crawshay-Williams, T. Schober, R. A. Floto, D. R. Spring. Unlocking Amides: A General Method for the Self-Immolative Release of Amide Containing Molecules. *Angew. Chem. Int. Ed.* **2024**, 63, e202402267. https://doi.org/10.1002/anie.202402267

J. D. Sydenham, H. Seki, S. Krajcovicova, L. Zeng, T. Schober, T. Deingruber, D. R. Spring. Site-selective peptide functionalisation mediated via vinyl-triazine linchpins. *Chem. Commun.* **2023**, 59, 706–709. https://doi.org/10.1039/D3CC05213C

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Dr Ruth Webster | click here for video

Chemistry at the interface with Biology and Medicine

Research in the Webster group sits at the boundary between organic and inorganic synthesis. We employ earth abundant metals in catalysis, with a specific focus on using designed iron catalysts in atom economic transformations. The complexities of iron catalysis require us to employ a range of different techniques, and work with collaborators with expertise in complimentary areas (such as DFT, EPR and advanced mass spectrometry techniques), to gain understanding of novel bond breaking and bond making processes.

We have a particular interest in the chemistry of phosphorus, and often couple this with iron catalysis to develop new transformations.

Relevant Papers

Synthetic and Mechanistic Studies into the Reductive Functionalization of Nitro Compounds Catalyzed by an Iron(salen) Complex, *J. Am. Chem. Soc.* **2024**, 146, 19839.

Synthesis and Characterization of a Terminal Iron(II)-PH_2 Complex and a Series of Iron(II)-PH_3 Complexes, *Inorg. Chem.* **2024**, 63, 6998.

The Complex Reactivity of $[(salen)Fe]_2(\mu\text{-}O)$ with HBpin and Its Implications in Catalysis, *ACS Catal.* **2023**, 13, 11841.

Taming PH_3: State of the Art and Future Directions in Synthesis, J. Am. Chem. Soc. 2022, 144, 16684.

An Iron-Catalyzed Route to Dewar 1,3,5-triphosphabenzene and Subsequent Reactivity, *Angew. Chem. Int. Ed.* **2022**, 61, 10.1002/anie.202208663.

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Physical Chemistry

Turning Phenomena into Quantitative Science

Physical Chemistry at Cambridge has two broad but overlapping aims.

One is to understand the properties of molecular systems in terms of physical principles. This work underpins many developing technological applications that affect us all, such as nanotechnology, sensors and molecular medicine.

The other is Atmospheric Chemistry (AC) where the interactions between chemical composition, climate and health are studied using a range of computer modelling and experiment based approaches. Together these two areas form a richly interdisciplinary subject spanning the full range of scientific methodologies: experimental, theoretical and computational. It is the research area with something for everyone.

If you are keen to work on a project in one of the Physical Chemistry groups, contact the group leader directly. Discuss your application with them in advance of submitting your formal application form to the University. The Physical Chemistry research groups accepting postgraduate students (PhD and MPhil) October 2025 are:

Prof. Alex Archibald

Prof. Stuart Clarke

Prof. Chiara Giorio

Prof. Sir David Klenerman FRS

Prof. Steven Lee

Prof. Stephen Jenkins

Prof. Tuomas Knowles

Professor Alex Archibald | click here for video

Modelling the Chemistry of the Atmosphere

In our team we study the chemistry of the gases and particles present in the air around us. We are concerned with understanding what is causing these compounds to change in their abundance and constitution and what are the impacts of these changes for human health, weather and climate. This interdisciplinary work requires chemists and physical scientists from a range of backgrounds to come together to help tackle some of these grand challenges. The bulk of the work in our team focusses on the use of numerical simulations using high performance computers (super computers). We are home to the UK National Centre for Atmospheric Sciences global model development team and provide bespoke support to our postgraduate students in running and analysing global model simulations.

Postgraduates from the group have gone on to work in a wide range of jobs in academia and industry, increasingly in the software/technology area.

Relevant papers:

Staniaszek, Z., Griffiths, P.T., Folberth, G.A., O'Connor, F.M., Abraham, N.L. and Archibald, A.T., The role of future anthropogenic methane emissions in air quality and climate. ***npj Climate and Atmospheric Science,*** **2022**, 5(1), pp.1-8.

Potential impacts of emissions associated with unconventional hydrocarbon extraction on UK air quality and human health, ***Air Quality, Atmosphere & Health,*** **2018,** *11*, 627.

Recent multivariate changes in the North Atlantic climate system, with a focus on 2005–2016, ***International Journal of Climatology,*** **2018,** *38,* **5050-5076.**

A world avoided: impacts of changes in anthropogenic emissions on the burden and effects of air pollutants in Europe and North America, ***Faraday Discussions,*** **2017**, *200*, 475.

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Professor Stuart Clarke | click here for video

In Depth Study of the Superficial

Our research centres on the behaviour of molecules adsorbing on to surfaces which is important in many areas, from batteries and supercapacitors to biological implants and making smooth ice cream. However, this is an experimental challenge because we are focussed on molecular monolayers which are 'buried' between two large amounts of bulk material, such as at the solid/liquid interface.

We have been developing a suite of approaches, including scattering methods at the world's leading synchrotron and neutron facilities, and an impressive suite of novel home-based physical, thermodynamic, spectroscopic and calorimetric methods.

Much of our work attracts industrial partners, and we often have iCASE awards which may involve a period working with an industrial partner at their premises. Present areas of interest include ions in solutions and at interfaces for batteries and supercapacitors, in-plane non-covalent interactions to determine the structures of adsorbed molecules for catalysis, lubricants under increasingly extreme conditions of temperature, pressure and imposed flow relevant for modern wind turbines and deposition in heat exchangers.

Relevant Papers

Wilson *et al*; **(2022)** Freezing fouling from aqueous solutions of TBAB and TME clathrate hydrates, ***accepted for Chem. Eng. Sci.***

Davidson *et al*, "2D Constraint Modifies Packing Behaviour: A Halobenzene Monolayer with X3 Halogen-Bonding Motif" ***Mol. Phys* (2021)**, e1900940 special edition.

Agrawal, *et al*, Novel semiconducting iron-quinizarin metal-organic framework for application in supercapacitors, ***Molecular Physics***, (**2019**), 117, 3424-3433.

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Professor Chiara Giorio | click here for video

Elucidating the Present and Past of the Atmosphere Using Analytical Tools

The atmosphere is a multiphase environment in which gases, particles and fog/cloud droplets interact. The chemical reactions happening in this complex environment can change the composition and the reactivity of atmospheric components and therefore their effects on the Earth's climate and on public health. We use a multifaceted experimental approach, combining field measurements and laboratory experiments, to understand the evolution of particles in the atmosphere, and assess their effects on climate and on public health. We work on developing methods using advanced analytical tools, from high-resolution mass spectrometry to top notch microscopy and spectroscopy techniques, together with multivariate data analysis. We use the fundamental information on particle reactivity and composition to reconstruct past compositional changes of the atmosphere from analysis of organic biomarkers in ice cores.

Relevant Papers

Prospects for reconstructing paleoenvironmental conditions from organic compounds in polar snow and ice. *Quaternary Science Reviews*, **2018**, 183, 1-22.

Formation of metal-cyanide complexes in deliquescent airborne particles: a new possible sink for HCN in urban environments. ***Environmental Science and Technology***, **2017**, 51, 14107-14113.

Cloud processing of secondary organic aerosol from isoprene and methacrolein photooxidation. ***Journal of Physical Chemistry A***, **2017**, 121, 7641–7654.

Online quantification of Criegee intermediates of α-pinene ozonolysis by stabilisation with spin traps and proton transfer reaction mass spectrometry detection. ***Journal of the American Chemical Society***, **2017**, 139, 3999-4008.

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Professor Sir David Klenerman FRS | click here for video

Watching Molecules in Action

The development of quantitative methods to directly observe individual molecules in solution, attached to surfaces, in the membrane of live cells or more recently inside live cells, has been a major advance in this last decade. We can now study how individual cellular components interact to form a cell and how this can go awry in disease.

My group (and collaborators) has focussed on developing these methods and applying them to biological/biomedical problems difficult or impossible to solve using conventional methods. We use scanning ion conductance microscopy for nanoscale imaging of live cells, controlled delivery of molecules to the cell surface and chemical mapping.

We have also developed single molecule fluorescence to detect interactions of molecules in the test-tube and on cells. These methods can be used to gain new molecular insights, as illustrated by our recent work on the role of proteins aggregates in neurodegenerative disease and the molecular basis of the immune response.

Relevant Papers

Nanoscopic Characterisation of Individual Endogenous Protein Aggregates in Human Neuronal Cells, ***Chembiochem,* 2018**, *19*, 2033.

Inhibiting the Ca2+ Influx Induced by Human CSF, ***Cell Rep,* 2017**, *21*, 3310.

Imaging and Characterisation of the Surface of Live Cells, ***Curr. Opin. Chem. Biol.,* 2011**, *15*, 696.

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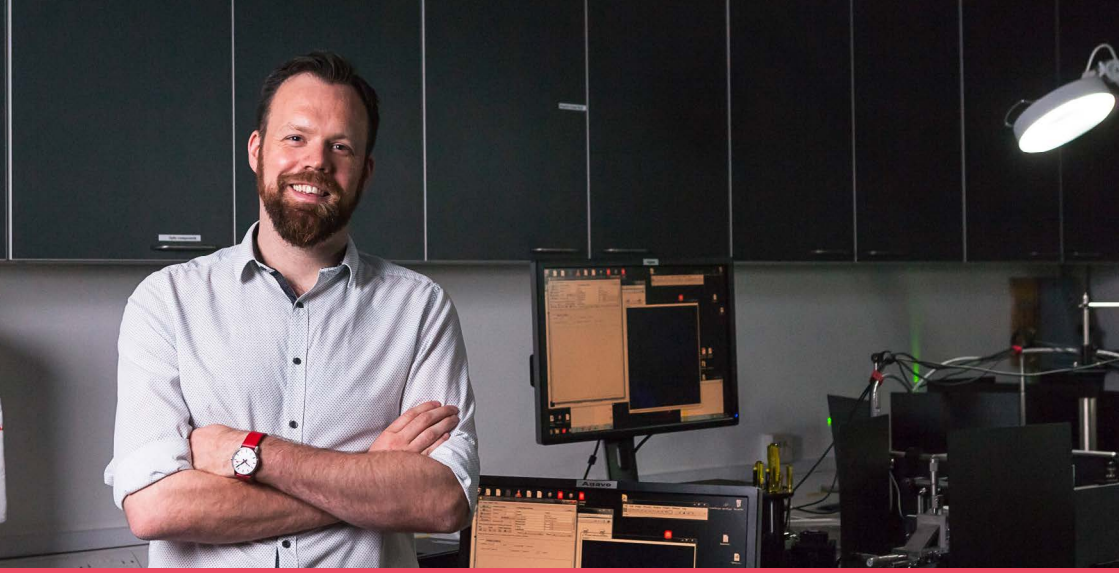

Professor Steven Lee | click here for video

Building New Tools to Study Single Molecules

Our research centres on building new tools to study single biomolecules using a variety of advanced ultrasensitive optical techniques, primarily through single-molecule fluorescence and super-resolution imaging techniques.

This requires an interdisciplinary combination of research skills including chemistry, physics, engineering and computational methods that synergistically come together to help answer 'real world' biological problems by directly visualising biological processes inside living cells as they unfold.

New projects include the technology of our newest 3D microscope, which works via a "double helix point spread function", the application of it to human immune cells, developing new dye molecules which will enable us to answer more challenging problems in the future, and imaging human brain for protein aggregates in Parkinson's disease.

Relevant Papers

Structure-specific amyloid precipitation in biofluids, ***Nat Chem*** **(2022)** doi: 10.1038/s41557-022-00976-3.

vLUME: 3D virtual reality for single-molecule localization microscopy, ***Nature Methods*** **(2020)** 17, 1097–1099

Multi-dimensional super-resolution imaging enables surface hydrophobicity mapping. Nature Communications (2016) 7, 13544

3D Structures of Individual Mammalian Genomes Studied by Single-cell Hi-C, ***Nature***, **(2017)**, 544

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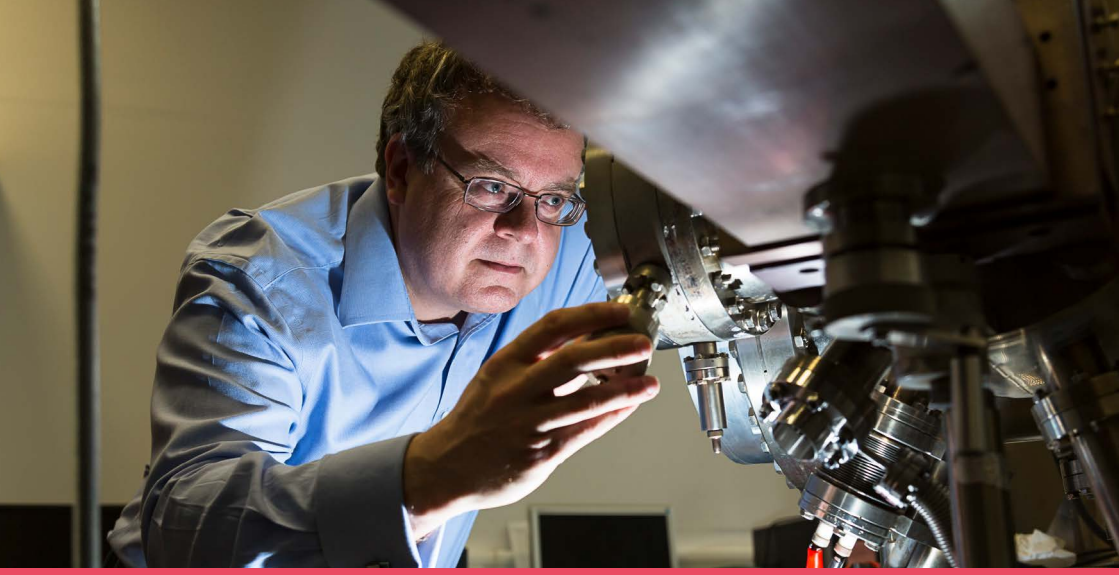

Professor Stephen Jenkins | click here for video

Symmetry, Structure and Dynamics in Surface Chemistry

Modern surface science provides unprecedented insight into physical and chemical processes relevant to sensing, corrosion and heterogeneous catalysis.

My group makes extensive use of first-principles modelling (density functional theory) linked strongly with experimental work conducted here and elsewhere. In this way, we gain understanding at the level of individual adsorbed molecules and individual reaction events, relating these to the underlying physical properties of the surface.

One major focus of our work is on the propagation of chirality between molecules and surfaces; another is on the dynamic processes of bond making and breaking that occur upon adsorption, desorption or surface reaction. In either case, the interplay between symmetry and the low-dimensional surface environment is of paramount importance.

Relevant Papers

First-Principles Dynamics of Fluorine Adsorption on Clean and Monohydrogenated Si{001}, ***Langmuir***, **2022**, 38, 7256.

The Dehydrogenation of Butane on Metal-Free Graphene, ***J. Colloid Interface Sci.***, **2022**, 619, 377.

Surface Chirality Influences Molecular Rotation upon Desorption, ***Phys. Rev. Lett.***, **2021**, 126, 166101.

Comparative Study of Single-Atom Gold and Iridium on CeO2{111}, ***J. Chem. Phys.***, **2021**, 54, 164703.

2D Constraint Modifies Packing Behaviour: A Halobenzene Monolayer with X3 Halogen-Bonding Motif, ***Mol. Phys.***, **2021**, 119, e1900940

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Professor Tuomas Knowles | click here for video

Biophysical Chemistry of Proteins

In order to be functional, most proteins have to associate with other proteins to form complexes, the molecular machinery of life. Moreover, incorrectly formed complexes are associated with a range of disorders, including Alzheimer's and Parkinson's diseases.

This supra-molecular behaviour of proteins is thus increasingly viewed as a key new frontier in biophysical chemistry, but one which is challenging to probe using conventional methods.

Current work includes the development and application of new biophysical methods for the study of protein behaviour. Physical chemistry can make a significant contribution to protein science, both through the development of novel measurement and analysis approaches.

Relevant Papers

Latent Analysis of Unmodified Bomolecules and their Complexes in Solution with Attomole Detection Sensitivity, *Nature Chem.*, **2015**, *7*, 802.

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Theoretical Chemistry

New Insights from Theory and Simulation

Theoretical chemistry is now one of the most thriving and exciting areas of chemistry. Our research covers a range of length and time scales, including active development of new theoretical and computational tools. Applications include high-res spectroscopy, atomic and molecular clusters, biophysics, surface science and condensed matter, complementing experimental research in the department.

We develop new tools for quantum and classical simulations and informatics, and investigate molecules using descriptions that range from atomic detail to coarse-grained models of mesoscopic matter. This work often begins with analytical theory, which is developed into new computer programs, applied to molecules and materials of contemporary interest, and ultimately compared with experiment.

If you are keen to work on a project in one of the Theoretical Chemistry groups, contact the group leader directly. Discuss your application with them in advance of submitting your formal application form to the University.

The Theoretical Chemistry research groups accepting postgraduate students (PhD and MPhil) for entry in October 2025 are:

Prof. Stuart Althorpe

Prof. Rosana Collepardo

Prof. David Wales FRS

Dr Robert Jack

Prof. Angelos Michaelides FRS

Dr Aleks Reinhardt

Dr Alexander Thom

Professor Stuart Althorpe | click here for video

Quantum Dynamics in Chemistry

Our research focusses on simulations of quantum dynamics (QD), i.e. quantum effects in the motion of atomic nuclei. These effects are challenging to simulate on the computer because they typically occur in the cross-over zone between quantum and classical mechanics (CM).

If the nuclei are heavy, one can get away with CM. But if they are light, the chemistry can be dominated by quantum effects e.g. quantum tunnelling can speed up rates of hydrogen-transfer reactions by orders of magnitude at rt, as can zero-point energy effects. Until recently, QD could only be done for very simple models, because solving the Schrödinger equation is otherwise impossible.

However, a number of recent breakthroughs now allow QD to be simulated in liquids and chemical reactions. The key is to exploit the near-classical behaviour of nuclei, by using techniques based on the Feynman description of quantum mechanics.

Relevant Papers

Concerted Hydrogen-bond Breaking by Quantum Tunneling in the Water, ***Hexamer Prism Science***, **2016**, *351*, 1310.

Which quantum statistics–classical dynamics method is best for water? R L Benson, G Trenins, and S C Althorpe *Faraday Discuss.* 221, 350-366 **(2020)**

Path-integral approximations to quantum dynamics. S C Althorpe. ***Eur. Phys. J. B.*** 94, 155 **(2021)** (17 pages)

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Professor Rosana Collepardo | click here for video

Multiscale Modelling of Genome Organization

One of the main challenges in genome biology is finding out how genomes function. Genomes have intricate 3D spatial organizations that are sensitive to the cell type and cell cycle stage, and that are intimately linked to function. By pushing the current limits of realistic computational modelling of chromatin and exploiting the advances in high-performance computing, our group is investigating a transformative new paradigm that suggests that nature uses the physical chemistry of phase separation – liquid-liquid phase separation – to control genome organisation and gene activity.

Our group develops multiscale models to investigate the unknown molecular mechanisms that dictate genome structure and dynamics, the role of liquid-liquid phase separation in genome organization, and the link between genome organization and function.

Relevant Papers

Emergence of Chromatin Hierarchical Loops from Protein Disorder and Nucleosome Asymmetry, *PNAS*, **2020**, 117, 7216-7224.

Liquid-Network Connectivity Regulates the Stability and Composition of Biomolecular Condensates with Many Components, *PNAS*, **2020**, 117, 13238-13247.

Oligonucleotides Can Act as Superscaffolds that Enhance Liquid-Liquid Phase Separation of Intracellular Mixtures, bioRxiv, **2020**: https://doi.org/10.1101/2020.01.24.916858

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Dr Robert Jack

Collective Behaviour in Soft Matter

Colloids, glasses, and gels are "soft matter"– in many cases, their properties lie somewhere between liquids and solids.

We aim to describe these materials using theory and computer simulation, concentrating on how the collective behaviour of many microscopic particles can give have unusual macroscopic consequences.

Examples include the spontaneous self-assembly of nano-scale structures and the formation of very stable glassy solids.

Relevant Papers

Statistical Mechanics of Dynamic Pathways to Self-assembly, ***Ann. Rev. Phys. Chem.***, **2015**, *66*, 143.
Investigating Amorphous Order in Stable Glasses by Random Pinning, ***Phys. Rev. Lett.,*** **2014**, *112*, 255701.

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Professor Angelos Michaelides FRS | click here for video

Fundamental Theoretical Studies of Key Global Challenges

Our research aims at understanding important phenomena in surface-, materials-, and nano-science. Using concepts from quantum mechanics to statistical mechanics, we apply and develop methods and computer simulations to study, for instance, surfaces, interfaces, and processes of environmental relevance.

Topics under consideration at present – for which PhD projects are currently available – include studies aimed at obtaining a molecular level description of water at interfaces, the application of state-of-the-art electronic structure methods to fundamental problems at surfaces and in materials, the development of machine learning potentials and fundamental studies in heterogenous catalysis.

Research projects in our group are generally highly collaborative involving e.g. international groups in the field and access to and exploitation of some of the largest supercomputers in the world.

Relevant Papers

Medium density amorphous ice, *Science*, **2023**, 379, 474.

The first-principles phase diagram of monolayer nano confined water, *Nature*, **2022**, 609, 512.

First-principles design of a single-atom–alloy propane dehydrogenation catalyst, *Science*, **2021**, 372, 1444.

Machine learning potentials for complex aqueous systems made simple, *PNAS*, **2021**, 118, e2110077118.

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Dr Aleks Reinhardt | click here for video

Phase Behaviour of Materials

We are a computational chemistry group working in the broad field of statistical mechanics. We are interested in the behaviour of various materials, from atomic and molecular to soft condensed matter and biological systems. In particular, we are interested in phase behaviour, nucleation and self-assembly. Quantifying bulk phase behaviour requires extensive sampling of phase space, which would be prohibitively expensive using first-principles methods. At the same time, understanding the dynamics of a process from a microscopic perspective is often beyond the reach of experiment. As a result, clever simulation methods are required to be able to study such processes, and we are interested in developing suitable techniques to tackle different systems.

Relevant Papers

Phase diagrams — Why they matter and how to predict them, *J. Chem. Phys.*, **2023**, 158, 030902. (Link: https://doi.org/10.1063/5.0131028)

Quantitative real-time in-cell imaging reveals heterogeneous clusters of proteins prior to condensation, *Nat. Commun.*, **2023**, 14, 4831. (Link: https://doi.org/10.1038/s41467-023-40540-2)

Quantum-mechanical exploration of the phase diagram of water, *Nat. Commun.*, **2021**, 12, 588. (Link: https://doi.org/10.1038/s41467-020-20821-w)

Direct observation and rational design of nucleation behaviour in addressable self-assembly, *Proc. Natl Acad. Sci. USA*, **2018**, 115, E5877. (Link: https://doi.org/10.1073/pnas.1806010115)

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Dr Alexander Thom | click here for video

Developing New Methodologies in Electronic Structure Theory

My research group develops and uses new methods to calculate the electronic structure of both molecular and solid-state systems, in order to tackle the challenging cases where existing methods fail, such as bond-breaking, electronic excited states, the description of molecular magnets, and strongly correlated solids.

We have three main focusses: tackling the scaling of highly accurate coupled cluster methods by using Monte Carlo sampling; designing algorithms which can exploit the power of present and future quantum computers for quantum chemistry; and designing computationally inexpensive methods for multi-reference systems as an alternative to CASSCF.

These methods usually involve writing new software and we use a range of programming languages: Fortran, C++ and Python, and exploiting massively parallel compute architectures, as well as GPUs and reprogrammable hardware (FPGAs), and quantum computers.

Relevant Papers

Reducing unitary coupled cluster circuit depth by classical stochastic amplitude prescreening. ***Phys. Rev. Res.*** 4, 023243 **(2022)** (link http://dx.doi.org/10.1103/PhysRevResearch.4.023243)

Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach. ***J. Chem. Theory Comput.*** 16, 5586 **(2020)** (link: http://dx.doi.org/10.1021/acs.jctc.0c00468)

A General Approach for Multireference Ground and Excited States using Non-Orthogonal Configuration Interaction. ***J. Chem. Theory Comput.*** 15, 4851, **(2019)** (link http://dx.doi.org/10.1021/acs.jctc.9b00441)

The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up.

J. Chem. Theory Comput. 15, 1728, **(2019)** (link http://dx.doi.org/10.1021/acs.jctc.8b01217)

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Professor David Wales FRS

Energy Landscapes

Our research involves exploration of energy landscapes, with applications to chemical biology, spectroscopy, clusters, solids, surfaces, and machine learning. We develop new theory and simulation tools in three main areas. First is structure prediction based upon global optimisation. Second is enhanced sampling, to predict thermodynamic properties, and understand how the quantities measured in experiments are related to the structure encoded by the potential energy surface. Third is the development of new methods to treat rare event dynamics, where we characterise the transition states and pathways that connect local minima.

New horizons have been opened up by more efficient methodology and faster computer hardware, with recent results for protein folding and misfolding, RNA and DNA, analysis and design of mesoscopic structures and materials, and condensed matter, including glassy systems and energy storage. All these techniques have now been brought to bear to characterise the prediction landscapes generated in machine learning, with diverse applications ranging from patient outcomes in hospital to geometry optimisation.

Relevant Papers

Exploring Energy Landscapes, ***Annu. Rev. Phys. Chem.***, **2018**, *69*, 401.

Exploring biomolecular energy landscapes, ***Chem. Comm.***, **2017**, *53*, 6974.

Energy landscapes for machine learning, ***Physical chemistry chemical physics***, **2017**, *19*, 12585.

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Biological Chemistry

Life is in the Chemistry Inside Each of Us

Biological Chemistry research at Cambridge focusses on understanding the chemistry of life, both the physical processes occurring at the molecular level and the chemical reactions.

The major themes amongst the Biological Chemistry groups are biological polymers, proteins and nucleic acids – how they interact with each other and with small molecules. How do proteins fold to a defined structure and why do they sometimes not fold causing neurodegenerative diseases? How do proteins catalyse reactions? Can we make small molecules that inhibit these processes? What structures can nucleic acids adopt? How can we detect and what is the role of modifications of individual nucleotides? How can we target medicinally active compounds where they are needed?

If you are keen to work on a project in one of the Biological Chemistry groups, contact the group leader directly. Discuss your application with them in advance of submitting your formal application form to the University.

The Biological Chemistry research groups accepting postgraduate students (PhD and MPhil) for entry in October 2025 are:

Prof. Sir Shankar Balasubramanian FRS

Dr Paul Barker

Prof. Gonçalo Bernardes

Dr Mateo Sanchez Lopez

Dr Pietro Sormanni

Prof. Michele Vendruscolo

Dr Julian Willis

Prof. Sir Shankar Balasubramanian FRS | video here

The Dynamic Chemistry, Structure & Function of DNA

There are new insights emerging about how DNA works that go beyond the classical view of the DNA double helix, Watson-Crick base pairing and the genetic code. My laboratory studies two new dimensions to DNA. The first is the existence of configurations that are not the Watson-Crick double helix, with a focus on four-stranded DNA structures called G-quadruplexes that can form in G-rich sequences in the test tube and within cells. The second is the study of natural, chemically modified DNA bases that give rise to a DNA alphabet that extends beyond G, C, T and A. The expanded chemistry of DNA is dynamic and can be altered in ways that shape the identity of cells and tissues, sometimes called epigenetic control.

We investigate the chemistry, structure, function and associated molecular mechanisms of these epigenetic bases, through experimental approaches ranging from chemistry to molecular biology and genomics. My group is split between two laboratories, one in the Yusuf Hamied Department of Chemistry and the other at the Cancer Research UK Cambridge Institute. We function together as an integrated unit with constant exchange of ideas, experimental approaches and people between the two sites.

Relevant Papers

Chem-map profiles drug binding to chromatin in cells, *Nature Biotechnology*, **2023**, 41, 1265.

The Structure and Function of DNA G-Quadruplexes, *Trends in Chemistry*, **2020**, 2:2, 123.

Detection, Structure and Function of Modified DNA Base, *J. Am. Chem. Soc.*, **2019**, 141, 6420.

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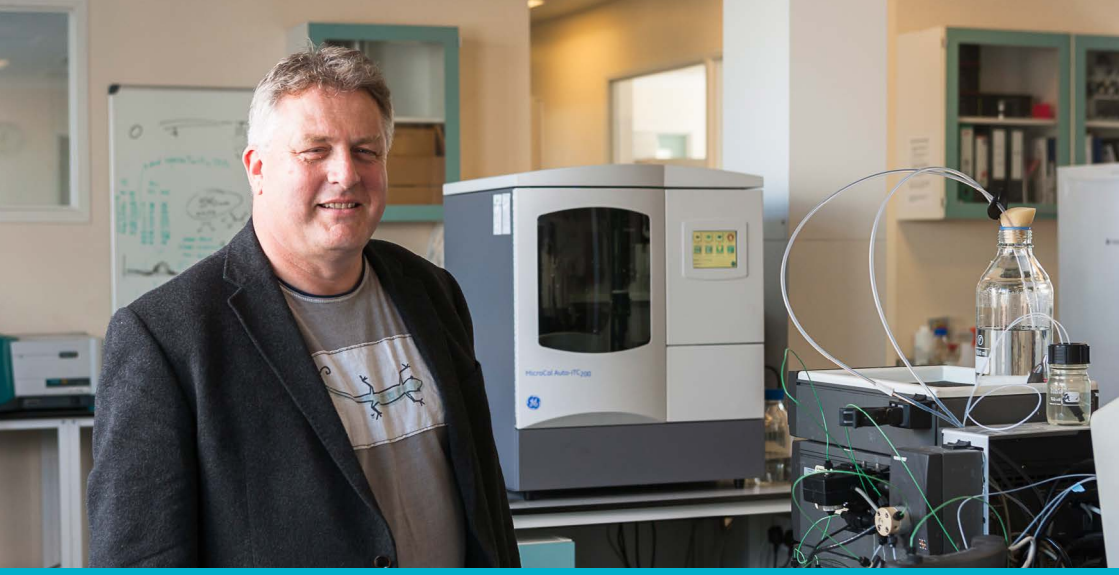

Dr Paul Barker | click here for video

Engineering Metalloproteins

The interplay between metal and protein chemistries is central to molecular biology. The intrinsic activities of metal ions are selectively tuned by binding to protein matrices; alternatively, protein structure is stabilised or altered upon metal ion binding.

By understanding the fundamentals of protein structure and dynamics, my group explores protein-metal binding sites through in vitro evolution and protein engineering combined with synthesis of novel metal complexes, including porphyrins.

We also examine the interaction between organometallic complexes and proteins, and the protein binding of ruthenium arena complexes has potential for medicinal applications. Through the generation of novel metalloprotein complexes, we aim to provide new materials for molecular electronic, catalytic, pharmaceutical and biosensing applications.

Relevant Papers

How to Make a Porphyrin Flip: Dynamics of Asymmetric Porphyrin Oligomers, ***Phys. Chem. Chem. Phys.***, **2015**, *17*, 27094.

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Professor Gonçalo Bernardes | click here for video

Translational Chemical Biology

A key aspect of my research group is the use of chemistry principles to develop molecules whose action is restricted to the tissue(s) where they should work to maximise therapeutic efficacy and reduce side-effects. Our 'bench to clinic' approach motivates us to work across disciplines, from organic chemistry to machine learning to immunology.

Recent examples of emerging areas in our group include the design of new chemistry for a) residue-specific modification of proteins and antibodies[1] and b) to bioorthogonally turn-on the activity of small-molecule drugs in vivo with methods based on metals and tetrazine-activation that expand the gamut of bond-cleavage reactions[2,3]. A key aspect of our research focuses on new drugs and targets. For example, we discovered that piperlongumine is an allosteric antagonist modulator of TRPV2 which leads to glioblastoma remissions in mice[4]. More recently, we reported RNA-degraders — a novel class of small molecules that degrade RNA[5], which we used to develop Click-Seq, a broad tool to edit and analyse known and unknown RNA modifications directly in cells.

The projects highlighted show how chemistry-driven approaches improve our understanding of complex biological phenomena that will inform the next generation of therapeutics.

Relevant papers:

[1]J. Am. Chem. Soc. **2018**, 140, 4004. [2]J. Am. Chem. Soc. **2020**, 142, 10869. [3]Angew. Chem. Int. Ed. **2020**, 59, 16023. [4]ACS Cent. Sci. **2021**, 7, 868. [5]ACS Cent. Sci. **2020**, 6, 2196.

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Dr Mateo Sanchez Lopez | click here for video

Developing new molecular tools for cell biology and neuroscience through chemical and synthetic biology

Having recently been awarded a Wellcome Trust Career Development Award to start an independent group in the department of chemistry at Cambridge in Oct 2023, our group works at the frontier between chemistry and biology. The research aims to apply the principles of chemistry in order to unlock our understanding of cell biology and using biology to create new chemistry. Specifically, we plan to develop new molecular tools leveraging optogenetics and protein engineering for cell biology and neuroscience. Another part of our research program will focus on the engineering of artificial metalloenzymes to catalyse new chemical reactions.

Relevant papers:

Sanchez MI, Wang W, Nguyen Q.-A, Soltesz I, Ting AY, *PNAS*, **2020**, 117, 33186.

Sanchez MI, Ting AY, *Nat. Methods*, **2020**, 17, 167.

Sanchez MI, Rama G, Calo R, Ucar K, Lincoln P, Vázquez López M, Melle-Franco M, Mascareñas JL, Vázquez ME., *Chem. Sci.*, **2019**, 10, 8681.

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Dr Pietro Sormanni | click here for video

Antibody Discovery by Rational Design

Antibodies are key tools to address questions and enable discoveries in biomedical research, and are increasingly employed to diagnose and treat many diseases, including cancer and neurodegeneration. By using a multidisciplinary approach that encompasses computational method development and in vitro experiments, we develop new data-driven technologies of rational antibody design at a computer. Our technologies are beginning to enable the discovery of antibodies against therapeutically relevant targets challenging to access with conventional approaches, and to provide novel time- and cost-effective alternatives. We also collaborate with the pharmaceutical industry and other academic groups in the Chemistry of Health, and we develop new antibodies for diagnostic applications.

Relevant papers

Fragment-Based Computational Design of Antibodies Targeting Structured Epitopes, *Science Advances*, **2022**, 8, eabp9540

Automated Optimisation of Solubility and Conformational Stability of Antibodies and Proteins, *Nature Communications*, **2023**, 14, 1937

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Professor Michele Vendruscolo | click here for video

Chemistry of Health: From bench to bedside

Our research is aimed at understanding the molecular origins of neurodegenerative disorders, including Alzheimer's and Parkinson's diseases, and at opening in this way novel opportunities for drug discovery to prevent, delay or treat these conditions. We have set up an interdisciplinary approach that brings together concepts and methods from chemistry, physics, engineering, genetics and medicine, using a combination of in silico, in vitro and in vivo approaches. This programme is based on the premise that physical and chemical sciences can provide relevant contributions to address biological questions to understand the normal and aberrant behaviours of proteins and their links with human disease. We are thus investigating the nature and consequences of the failure to maintain protein homeostasis, and its association with ageing and neurodegenerative disorders.

We carry out this programme in the recently established Centre for Misfolding Diseases, which is hosted in the new Chemistry of Health building, which includes also the Chemistry of Health Incubator for translational research, and the Molecular Production and Characterisation Centre, a shared facility for research in chemical biology.

Relevant Papers

Drug discovery: S. Chia et al. SAR by kinetics for drug discovery for protein misfolding diseases. Proc. Natl. Acad. Sci. USA 115, 10245-10250 **(2018)**

Antibody design: F. A. Aprile et al. Rational design of a conformation-specific antibody for the quantification of Abeta oligomers. Proc. Natl. Acad. Sci. USA, 117, 13509-13518 **(2020)**.

Structural biology: M. Bonomi and M. Vendruscolo. Determination of protein structural ensembles using cryo-electron microscopy. Curr. Op. Struct. Biol. 56, 37-45, **(2019)**.

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Dr Julian Willis | click here for video

Synthetic Biology and Gene Editing

We are a new synthetic biology, molecular biology and biotechnology-focused research group. The common theme across our scientific work is exploring natural diversity to identify proteins with novel functions or properties, studying and characterising them, and finally engineering them to create new technologies.

Our main research focus is to study the DNA replication machinery of viruses and exploit them to develop new tools for gene editing and synthetic biology applications.

We study a fascinating and unusual class of viruses which use a unique mode of protein-primed DNA replication to replicate their linear DNA genomes. These represent one of the few known biological systems in which protein-DNA covalent bonds can be naturally found. This group of viruses are very understudied but hold great promise for exciting biotechnology applications. In particular, we are exploring how to repurpose these viral replication proteins to create innovative new tools for gene editing to treat human genetic disease.

Relevant Papers

Gene editing overview: AV Anzalone *et al.* (**2020**) Genome editing with CRISPR–Cas nucleases, base editors, transposases and prime editors. *Nat Biotechnol.* 38:824-844

Synthetic biology concepts: CC Liu *et al.* (**2018**) Toward an orthogonal central dogma. *Nat Chem Biol.* 14:103-106

Viral DNA replication system: M Salas *et al.* (**2016**) DNA-binding proteins essential for protein-primed bacteriophage Φ29 DNA replication. *Front Mol Biosci.* 3:37

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Group Lab Tour Videos

Yusuf Hamied Department of Chemistry, University of Cambridge

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