46th CCP5 Annual General Meeting 2026
Timetable & Programme | 9–11 September 2026
Venue: 2.07 – Yew Lecture Theatre, 2nd Floor, Nucleus Building, Edinburgh

INVITED Invited TALK Talk BREAK Break POSTERS Posters DINNER Dinner MEETING Meeting CHAIR Chair

Dinner: Thu Sep 10, 19:00 Hotel du Vin
Committee: Dr E. Ricci, Prof C. McCabe, Dr C. Hobday, Dr A. Elena
Web: https://agm46.ccp5.ac.uk **Wi-Fi:** Eduroam

September 9, 2026 – Day 1

12:00 – 13:00	LUNCH Arrival, Registration & Lunch
13:00 – 15:00	SESSION 1 **Chair:** Eleonora Ricci
13:00 – 13:15	WELCOME **Prof Chris Lorenz** - CCP5 Chair, King's College London - Welcome and Introduction
13:15 – 14:00	INVITED TALK **Prof David Wales** *(University of Cambridge)* Energy landscapes: Exploration and Discovery
14:00 – 14:20	TALK **Peter Cummings** *(Heriot-Watt University)* Achieving Reproducibility and Replicability of Molecular Dynamics and Monte Carlo Simulations Using the Molecular Simulation Design Framework (MoSDeF)
14:20 – 14:40	TALK **Nasser Afify** *(University of Edinburgh)* Multiscale Atomistic Simulation of Energy Materials and Processes — Limitations and Opportunities
14:40 – 15:00	TALK **Elliott Kasoar** *(STFC/University of Cambridge)* ML-PEG: ML Performance and Extrapolation Guide
15:00 – 15:30	BREAK Coffee Break
15:30 – 16:55	SESSION 2 **Chair:** Alin Elena
15:30 – 16:15	INVITED TALK **Prof Maria Grazia De Angelis** *(University of Bologna)* Bridging AI and Physics-Based Models for Predicting Material Separation Performance
16:15 – 16:35	TALK **Leo Lue** *(University of Strathclyde)* A gradient density functional theory for self-assembling molecular systems
16:35 – 16:55	TALK **Lois Smith** *(University of Liverpool)* PolyRapid: Automated High-Throughput Screening of Polymers Using a Computational Workflow
16:55 – 18:30	POSTERS Poster Session

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September 10, 2026 – Day 2 (Morning: Sessions 3 & 4)

09:00 – 10:45	SESSION 3 **Chair:** Andrew Logsdail
09:00 – 09:45	INVITED TALK **Prof Ed Maginn** *(University of Notre Dame)* Thermal Conductivity of Ionic Liquid Mixtures: From Nanostructure to Accurate Molecular Simulation
09:45 – 10:05	TALK **Mazin Saad Almarashi** *(Heriot-Watt University)* Using molecular simulations to examine the interaction of permeation enhancers with the skin barrier
10:05 – 10:25	TALK **Stephen Yeandel** *(University of Bristol)* Computational Insights into Phase Stability and Surface Segregation in GLO
10:25 – 10:45	TALK **Miguel Jorge** *(University of Strathclyde)* Quantifying uncertainty in experimental and simulated adsorption in Metal-Organic Frameworks
10:45 – 11:15	BREAK Coffee Break
11:15 – 12:35	SESSION 4 **Chair:** Clare McCabe
11:15 – 11:35	TALK **Panagiotis Kourtis** *(Newcastle University)* Applications of MACE Foundational Models on Battery Electrolytes
11:35 – 11:55	TALK **Marco Mattia** *(University of Edinburgh)* Learning kinase conformation across activation
11:55 – 12:15	TALK **Sarah Stewart** *(University of Edinburgh)* Amino Acid – Clay Interactions on Mars-Relevant Minerals
12:15 – 12:35	TALK **Stepan Zhikharev** *(University of Warwick)* chirality-kit: A stand-alone topology generator for functionalised and solvated nanostructures.
12:35 – 13:35	LUNCH Lunch

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September 10, 2026 – Day 2 (Afternoon & Dinner: Sessions 5 & 6)

13:35 – 15:20	SESSION 5 **Chair:** Chris Lorenz
13:35 – 14:20	INVITED TALK **Dr James Ewen** *(University of Bath)* Molecular Simulations of Interfacial Processes
14:20 – 14:40	TALK **Michael Seaton** *(UKRI STFC Daresbury Laboratory)* Polarising highly coarse-grained water for aqueous electrolytes
14:40 – 15:00	TALK **Rhys Blaney** *(The University of Strathclyde)* Quantifying Force Field Uncertainty for Biogas Upgrading in Zeolites
15:00 – 15:20	TALK **Asal Azar** *(University of Edinburgh)* Allosteric Regulation of Nitrite Reductase AniA Trimerisation by Copper Binding
15:20 – 15:50	BREAK Coffee Break
15:50 – 17:30	SESSION 6 **Chair:** Claire Hobday
15:50 – 16:10	TALK **Karen Johnston** *(University of Strathclyde)* A Molecular Dynamics Seeding Approach to Determine Critical Nucleus Size and Concentration for Crystal Nucleation
16:10 – 16:30	TALK **Amro Mohamed** *(Heriot-Watt University)* Computational Screening of Lignin-Derived Epoxy Networks for Gas Separation
16:30 – 16:50	TALK **Jasmine Lightfoot** *(STFC Hartree Centre)* From atoms to application: scalable simulation-driven formulation design
16:50 – 17:10	TALK **Joseph Thomas** *(Northumbria University)* Uncovering Ion Transport Pathways in High-Temperature Green Hydrogen Electrolyser Membranes via Machine-Learned Interatomic Potentials
17:10 – 17:30	TALK **Vanessa Ward** *(Durham University)* Understanding Correlated Motion is Critical to Accurate Predictions of Ionic Conductivity
19:00 – 22:00	DINNER **Conference Dinner** - Hotel du Vin - 11 Bristo Place, Edinburgh, EH1 1EZ

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September 11, 2026 – Day 3 (Sessions 7 & 8)

09:00 – 10:45	SESSION 7 **Chair:** Colin Freeman
09:00 – 09:45	INVITED TALK **Prof Tell Tuttle** *(University of Strathclyde)* Peptides at the Edge: Designing Function at Mineral and Ice Interfaces
09:45 – 10:05	TALK **Umberto Terranova** *(University of Buckingham)* Iron – Sulfur Cluster Redox Potentials Across Biological Scales
10:05 – 10:25	TALK **Duncan Dockar** *(University of Edinburgh)* Are bulk nanobubbles stabilised by contaminant surfactants?
10:25 – 10:45	TALK **Werner Muller** *(IFP Energies nouvelles)* Developing a Novel Coarse-Grained Force Field for Polyvinyl Chloride: Viscosity Predictions and Uncertainty Quantification
10:45 – 11:15	BREAK Coffee Break
11:15 – 12:45	SESSION 8 **Chair:** Paola Carbone
11:15 – 11:35	TALK **Andrew Logsdail** *(Cardiff Catalysis Institute, Cardiff University)* Developing new catalysts for CO_2 hydrogenation to fuels through multiscale computational modelling
11:35 – 11:55	TALK **Joseph Burke** *(Imperial College London)* Coarse-grained modelling of porous materials discovery
11:55 – 12:15	TALK **Andreas Hermann** *(The University of Edinburgh)* Atomistic modelling challenges for metal superhydrides
12:15 – 12:35	TALK **Shubham Deshpande** *(Heriot-Watt University)* Investigating the effects of ceramide variation on lipid organisation in the stratum corneum from molecular dynamics simulations
12:35 – 12:45	CLOSING Closing Remarks
12:45 – 14:00	LUNCH Lunch and Departure MEETING *Parallel CCP5 Exec Committee Meeting*