CCP5

Collaborative Computational Project

Computer Simulation of Condensed Phases

45th CCP5 International Conference and AGM

University of Liverpool

8th–10th September 2025

RSC INTEREST GROUP
STATISTICAL MECHANICS & THERMODYNAMICS

HENRY ROYCE INSTITUTE

UNIVERSITY OF LIVERPOOL

Welcome to Liverpool for the 45th CCP5 International Conference and Annual General Meeting.

We're delighted to welcome you to this event to celebrate the breadth of research across our community and foster new connections.

The conference is hosted by the School of Engineering. All talks will take place in the Hele-Shaw Lecture Theatre, while lunches and the poster session will take place in the Mason Bibby Common Room.

While you are here, we encourage you to visit the Victoria Gallery and Museum, located next to the Harrison Hughes Building. This is the original red brick building that gave its name to the group of UK universities established in the late 19th and early 20th centuries.

Our conference dinner will be held at Hope Street Hotel, approximately a 10-minute walk from the Harrison Hughes Building. Please see the map below.

Conference Organisers:
Aaron Finney, *School of Engineering, University of Liverpool*
Dmytro Antypov, *Leverhulme Centre for Functional Materials Design, University of Liverpool*
Alin Elena, *STFC Daresbury Laboratory*

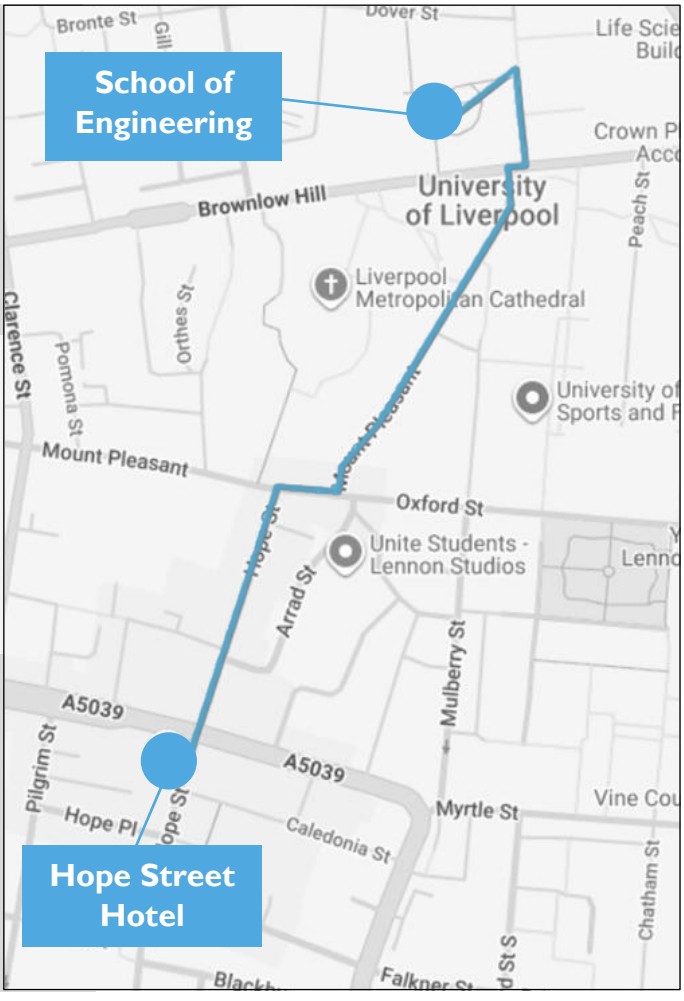
Wifi Login:

Eduoroam

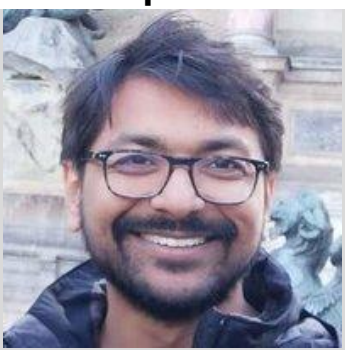
Guest UoL

Campus Map:

Liverpool Tourist Map:



Invited Speakers



Paramvir Ahlawat, *University of Cambridge*
Paramvir is currently based in the Optoelectronics Group at the Cavendish Laboratory. His research focuses on applying machine learning models to understand the morphological evolution and thermal properties of halide perovskites, supporting their rapid industrialisation. This builds on his PhD at EPFL (2022), studying crystallisation and phase transitions in perovskite solar cells, collaborating closely with the Michele Parrinello and Michael Grätzel groups.

Denis Andrienko, *Max Planck Institute for Polymer Research*
Denis is a group leader in theory and simulations of charge and exciton transport in organic semiconductors. He holds two PhDs from the Institute of Physics, Kiev, and University of Bristol, UK. He joined MPI-P as a Humboldt Fellow performing theoretical studies of the slippage effect, mechanical properties of polyelectrolyte microcapsules, and many-body interactions in soft systems.

Livia Bartók-Pártay, *University of Warwick*
Livia is an Associate Professor of Computational Chemistry specialising in atomistic simulations of molecular systems, with a focus on phase transitions and the prediction of stable crystalline structures. Her work includes developing computational methods and modelling nanochemical systems such as surfaces, interfaces, and adsorption phenomena, particularly at the liquid–vapour interface.

Marcus Campbell Bannerman, *University of Aberdeen*
Marcus is a Senior Lecturer in Engineering and works on a broad range of topics ranging from computational thermodynamics, particle dynamics simulation, and pilot-scale production trials of novel cement formulations to the virtual reality rendering of volumetric datasets and GPU programming. At the heart of it all is the development of engineering simulation software. Marcus was awarded the CCP5 Prize in 2024.

Doug Cleaver, *Sheffield Hallam University*
Doug is a Professor of Materials Modelling and was Mike Allen's first PhD student and then went on to post-doc with Dominic Tildesley. Since joining SHU, over 30 years ago, Doug has run numerous simulation-based studies of soft matter systems and, where necessary, developed innovative models and methodologies. He has a specific expertise on liquid crystals and interfacial interactions, but has also studied bicontinuous phases, polymer nanocomposites and complex, multi-generation self-assembly.

Stephen Cox, *Durham University*

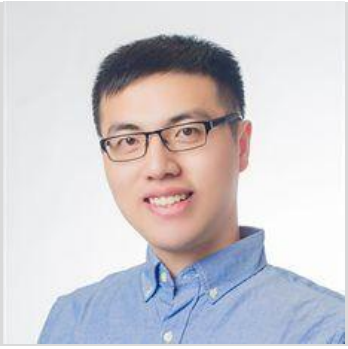
Stephen is an Assistant Professor in Computational Chemistry and Data Science, and a Royal Society University Research Fellow. His research combines theory and molecular simulation to study complex interfacial systems, such as crystal surfaces in solution, water–graphene interfaces, and electrode–electrolyte boundaries. He is particularly interested in developing classical density functional methods to understand how features at the microscopic scale impact mesoscopic phenomena.

James Elliott, *University of Cambridge*

James is a Professor of Macromolecular Materials Science and is soon to be the ex-Head of Department of Materials Science & Metallurgy at Cambridge. His research focusses on polymers and carbon nanomaterials, with a particular emphasis on energy and sustainability. As Director of the EPSRC CDT in Computational Methods for Materials Science (2017–2023), he coordinated doctoral training programmes for over 50 PhD researchers and co-created two new MPhil programmes in scientific computing and energy materials.

Kim Jelfs, *Imperial College London*

Kim is a Professor of Computational Materials Chemistry. Her group specialises in the use of computer simulations and artificial intelligence to assist in the discovery of supramolecular materials, particularly porous materials and organic electronics, working closely with experimental collaborators. She is co-Director of the Institute for Digital Molecular Design and Fabrication at Imperial, Co-Director of AIChemy, the EPSRC AI hub for Chemistry, and an Associate Editor for Chemical Communications.



Xiaocheng Shang, *University of Birmingham*

Xiaocheng Shang is an Associate Professor in Mathematical Optimisation and Data Science, with research focused on designing numerical methods for stochastic differential equations and their applications across mathematics, physics, and data science. He has held fellowships from The Alan Turing Institute, the LMS (Emmy Noether Fellowship), and EUniWell. Xiaocheng was the winner of the 2024–25 CECAM/CCP5 Sandpit award.

Programme

Date/Time	Activity/Speaker	Details/Title
8th September, Day 1		
12:00 - 13:00	Arrival and Registration	Harrison Hughes Reception, School of Engineering
13:00 - 13:15	Welcome	Hele Shaw Lecture Theatre
13:15 - 14:00	Livia Bartok-Partay, *University of Warwick*	Surface Phase Diagrams: Insights from Nested Sampling
14:00 - 14:25	Ian Rouse, *University College Dublin*	NPCoronaPredict: A Multiscale, Coarse-Grained Software Pipeline for Predicting the Nanoparticle-Biomolecule Corona
14:25 - 15:10	Stephen Cox, *Durham University*	Going Beyond Molecular Simulations with Neural Functional Theory
15:10 - 15:40	Coffee Break	Hele Shaw Lecture Theatre
15:40 - 16:25	Marcus Campbell Bannerman, *University of Aberdeen*	Event-Driven Molecular Dynamics and the Search for Anomalous Thermal Conduction
16:25 - 16:50	Murat Ozlek, *University College London*	Interfacial Phonon Bridging in Interlocked Graphene/Graphite Structures: A Combined Experimental and Machine Learning-Driven Simulation Study
16:50 - 17:15	Vanessa Ward, *Durham University*	A Rule That's Made to be Broken? Reframing the Arrhenius Law and the Calculation of Activation Energies for Ion Transport in Solid Electrolytes.
17:15 - 17:40	Samuel Ericson, *University of Manchester*	Coupling Micro-Mechanical and Molecular Models to Optimize Polymer Composites
17:40 - 19:30	Poster Session	Mason Bibby Common Room
9th September, Day 2		
09:00 - 09:45	James Elliot, *University of Cambridge*	Mesoscale Simulations of Ionomer Membranes
09:45 - 10:10	Amali Galappaththi Guruge, *University of Liverpool*	Computational Insights into Structural Changes in PEODT:PSS Interfaced with Water
10:10 - 10:35	Ajeeth Kanagarajan, *Durham University*	Investigating Negative Chemotaxis of Polymeric Vesicles using Multiscale Simulation Methods
10:35 - 11:00	Coffee Break	Hele Shaw Lecture Theatre
11:00 - 11:45	Xiaocheng Shang, *University of Birmingham*	Stochastic Norton Dynamics: An Alternative Approach for the Computation of Transport Coefficients in Dissipative Particle Dynamics
11:45 - 12:10	Adri Escañuela-Copado, *University of Granada*	Modelling Homo- and Co-Polymer Nanocomposites Including Nanodimers and Nanorods via Molecular Dynamics

12:10 - 12:30	Paola Carbone, CCP5 Chair	AGM News and Business
12:30 - 13:30	Lunch	Mason Bibby Common Room
13:30 - 14:15	Paramvir Ahlawat, *University of Cambridge*	Approaching Precise Large Scale All-Atom Simulations of Crystallisation of Halide Perovskites
14:15 - 14:40	Matteo Paloni, *University College London*	Unravelling Nucleation in Ferritin Nanocages from Atomistic Molecular Dynamics Simulations
14:40 - 15:05	Cillian Cockrell, *Bangor University*	The Effect of Impurities and Irradiation on the Glass Network – Cs_2O-loaded Iron Phosphate Case Study
15:05 - 15:30	Xue Yong, *University of Liverpool*	Computational Studies on Carbon Nitride-Supported Metals for the Selective Oxidation of HMF to DFF
15:30 - 16:00	Coffee Break	Hele Shaw Lecture Theatre
16:00 - 16:45	Denis Andrienko, *Max Planck Institute for Polymer Research*	Predicting Molecular Ordering in Deposited Molecular Films
16:45 - 17:10	Eleonora Ricci, *University of Edinburgh*	Combined Molecular and Data-Driven Modelling of Polymer Separation Membranes
17:10 - 17:35	Khadija Asif, *University of Strathclyde*	Evaluating Force Field and Water Model Effects on CO_2 Adsorption Predictions for Direct Air Capture using Metal-Organic Frameworks
19:00 - 22:30	Conference Dinner	Hope Street Hotel
10th September, Day 3		
09:00 - 09:45	Kim Jelfs, *Imperial College London*	Remembering the Lab in Computational Molecular Materials Discovery
09:45 - 10:10	Elliott Kasoar, *STFC and University of Cambridge*	Digital Infrastructure for Machine Learnt Interatomic Potentials
10:10 - 10:35	Wenkai Zhang, *STFC*	PSDI - What can we do for you
10:35 - 11:00	Coffee Break	Hele Shaw Lecture Theatre
11:00 - 11:45	Doug Cleaver, *Sheffield Hallam University*	Simulations Behaving Badly
11:45 - 12:10	Harvey Devereux, *Queen Mary University of London*	Calculating System Properties on the fly in DL_POLY 5
12:10 - 12:35	Gabriell Bramley, *Cardiff University*	Introducing EmbASI: A Re-usable, General Library for QM-in-QM Embedding
12:35 - 14:00	Lunch and Departure	Mason Bibby Common Room

Poster Presentations

Abdullah Al Rammah	*University of Manchester*	Limitations of Classical Force Fields for CO_2 Adsorption in MOFs: Toward Quantum Accuracy at DAC-Relevant Pressures
Miltiades Angelides	*University of Manchester*	TBC
Vivian Barron	*AWE*	AWE Materials Modelling For Ageing and Lifetime Predictions
Jose Javier Burgos-Marmol	*Unilever*	Equilibrium Surface Tension using Dissipative Particle Dynamics simulations
Matthew Carruthers	*University of Strathclyde*	Member and recipient of CCP5 funding for undergraduate summer bursary.
Shayan Doust	*University of Liverpool*	TBC
Joseph Flitcroft	*University of Manchester*	Predicting Infrared and Raman spectra using first principles modelling
Colin Freeman	*University of Sheffield*	Stability of Calcium Carbonate Nanoparticles
Varnit Jain	*University of Liverpool*	Optimising battery electrolytes
Keran Jiao	*University of Manchester*	A Computational Screening Study of N-donor based MOFs for High Temperature Ammonia Adsorption
Carlos Mendoza	*Instituto de Investigaciones en Materiales, UNAM*	Edge-on anchored discotic liquid crystals in spherical shells: A computational study of the phases and defects
Benjamin Mitchell	*University of Strathclyde*	Molecular Dynamics Simulation of Monoglyceride-Induced Bilayer Destabilisation in Model Membrane Systems
Oliver Morris	*Cardiff University*	Computational Modelling of Acid Zeolite Catalysed Dimethylnaphthalene Synthesis
Ciarán O'Brien	*STFC-SCD and University of Liverpool*	Modelling Electrocatalysts at a Charged Interface to Support the Interpretation of Nonlinear Vibrational Spectroscopy
Jokubas Pelanskis	*The University of Cambridge*	Modelling of ionomer thin films using many-body dissipative particle dynamics
Daniel Salgado	*Instituto Potosino de Investigación Científica y Tecnológica, AC.*	Monte Carlo simulation of a Discotic Liquid Crystal Shell with Mixed Anchoring Conditions
Jessica Steele	*University of Manchester*	Active Learning for Predicting Polymer/Plasticizer Phase Behaviour
Daniel Valero	*University of Granada*	Conductivity of polymer nanocomposites filled with polarisable nanorods under a DC electrical field

Yuhan Wang	*UCL*	Predictive Model Building for Aggregation Kinetics Based on Molecular Dynamics Simulations of an Antibody Fragment
Myles Ward	*University of Cambridge*	Non-Fluorinated Hydrocarbon Membranes for PEM Cells
Chin Yong	*STFC*	DL_FIELD – a software workflow tool for force field models.
Maryam Zarghamidehaghani	*University of Edinburgh*	Redefining hemodialysis with data-driven materials innovation: towards miniaturization and the wearable artificial kidney
Stepan Zhikharev	*Warwick Centre for Predictive Modelling*	Ionic Permittivity in Carbon Nanotubes: Re-examine the Role of Polarisability