6th CCPBioSim/CCP5 Multiscale Modelling Conference

Programme

Monday Afternoon – https://ukri.zoom.us/j/99655158845
Tuesday Morning – https://ukri.zoom.us/j/91045594839
Tuesday Afternoon – https://ukri.zoom.us/j/92992230968
Wednesday Morning – https://ukri.zoom.us/j/92212955259

Day 1 - Monday 31 March 2025

12:00 – 13:20	Registration and Lunch
13:20 – 13:30	**Welcome / Introduction (Session Chair: Marc van der Kamp)**
13:30 – 14:05	Alessandro Troisi *High-throughput screening of polymeric semiconductors*
14:05 – 14:25	Kirill Zinovjev *QM/MM without QM: electrostatic machine learning embedding for enzymatic catalysis, ligand binding and more*
14:25 – 14:45	Anna Bui *Learning classical density functionals for ionic fluids*
14:45 – 15:05	Edoardo Donadoni *The impact of polymer coating on nanoparticles interaction with lipid membranes explored by coarse-grained molecular dynamics simulations*
15:05 – 15:35	**Coffee**
15:35 – 16:10	Chantal Valeriani *From active polymers' assembly to mechanical properties of a bacterial biofilm*
16:10 – 16:30	Carlo Fonte *From Electrons to Reactors: ab initio multi-scale simulation of methane oxidation over palladium oxide*
16:30 – 17:00	*Flash Talks A*
17:00 – 18:30	**Poster Session A - Odd Numbers**

Day 2 - Tuesday 1 April 2025

08:30 – 09:00	**Coffee (Session Chair: Charlie Laughton)**
09:00 – 09:35	Matthias Schmidt *Neural functionals and unexpected symmetries in statistical mechanics*
09:35 – 09:55	Marko Hanzevacki *Reaction mechanism of choline degradation by choline trimethylamine-lyase (CutC) revealed with QM/MM modelling*
09:55 – 10:30	Lorna Dougan *Current challenges and opportunities in translating the mechanical properties of biomolecules across lengthscales*
10:30 – 11:05	**Coffee**
11:05 – 11:40	Katarzyna Swiderek *Deciphering the role of protein electrostatic field in enzymatic catalysis: A case study of three distinct heterogeneous Proteasome □-subunits*

11:40 – 12:00	Tom Headen *Wide Q-range Total Neutron Scattering: Simulation Based Data-Refinement for Multi-Scale Systems*
12:00 – 13:30	**Lunch (Session Chair: Paola Carbone)**
13:30 – 14:05	Valentina Erastova *Let's talk about dirt: from environmental sorptive materials of Earth to biosignatures in Space*
14:05 – 14:25	Maria Grazia De Angelis *Multiscale and machine learning-assisted models for the design of materials supporting net zero, energy transition, and circular economy*
14:25 – 14:45	Mark Miller *Superselectivity and Nucleation in Biomolecular Condensates*
14:45 – 15:15	**Coffee**
15:15 – 15:50	Rebecca Wade *Multi-resolution molecular simulations to investigate the interplay between cytochrome P450 interactions, conformational variability and function*
15:50 – 16:10	Alberto Pérez de Alba Ortíz *Novel Bayesian approaches to biomolecular free-energy calculations: from ion-responsive polysaccharide rigidities to nanoplastic-induced protein dissociation*
16:10 – 17:00	*Flash Talks B*
17:00 – 18:30	**Poster Session B – Even Numbers**
19:00	**Conference Dinner**

Day 3 - Wednesday 2 April 2025

08:30 – 09:00	**Coffee (Session Chair: Stephen Cox)**
09:00 – 09:35	Benedetta Mennucci *Multiscale strategies to investigate light-responsive proteins*
09:35 – 09:55	Thomas Sayer *Small polaron transport in very large lattices with accurate numerics*
09:55 – 10:15	You Lu *Py-ChemShell's Biomolecular Simulation Workflow and Recent Advances*
10:15 – 10:35	*Jean-Marc Lude* *Molecular Density Functional Theory with Atomistic Dipolar Solvent to Study Pressure Effect on a Diels-Alder Reaction*
10:35 – 11:05	**Coffee**
11:05 – 11:25	Shakir Ali Siddiqui *Local Electric Field-Guided Redox Potential Tuning in de novo Proteins*
11:25 – 11:45	Dmitry Nerukh *Upscaling Simulations: Integrating Molecular Dynamics with Hydrodynamics*
11:45 – 12:20	Jochen Blumberger *Simulating Electronic Quantum Dynamics on the Nanoscale (10-100nm)*
12:20 – 14:00	**Lunch and Close**

Posters With Prizes Sponsored by the RSC Journals

Poster Number	Presenter Name	Poster Title
1	Baumhauer, Fiona	Predicting azeotropic phase diagrams using machine learned classical density functional theory
2	Brukhno, Andrey	Shapespyer: a Python driven toolchain for soft matter simulations
3	Chattopadhyay, Rajorshi	Development of polarizable force field for La3+ in Cl-bearing hydrothermal fluids
4	Doveiko, Daniel	Binding Energy Calculations of Anthracene and Rhodamine 6G H-type Dimers: A Comparative Study of DFT and SMD Methods
5	Epstein, Alexander	Understanding Hydrophobicity in Complex Geometries via Classical Density Functional Theory
6	Fairchild, Connie	A Minimal Model for the Frequency-Dependent Conductivity of Ionic Liquids
7	Findlay, Elliot	Modelling Soil-release Polymers on Fabric Surfaces: Multiscale Insights from Dissipative Particle Dynamics and Enhanced Sampling MD Simulations
8	Fitkin, Arielle	A computational investigation of metal-organofluorine interactions and their role in selective metal deposition
9	Freeman, Colin	Mineral Control over Molecular Binding and Decay
10	Galappaththi Guruge, Amali	Computational insights into structural changes in PEODT:PSS interfaced with water
11	Gopalakrishna Rao, Aditya	Multiscale simulations of the mechanism of a de novo designed Diels Alderase photoenzyme catalysing [2+2] cycloadditions: implications for photobiocatalyst design
12	Hayton, John	Silver Iodide in Water – A Machine Learned Interatomic Potential with Electrostatics
13	Hodala, Aydin	The effect of aggregation on the pKa of oleic acid
14	Jia, Hengjian	Discovering Blood Brain Barrier Permeable Compounds

		with Cliques Descriptors
15	Igaev, Maxim	Microtubule dynamics are defined by conformations and stability of clustered protofilaments
16	Kanagarajan, Ajeeth	Negative Chemotaxis of polymeric vesicles against lactic acid concentration gradient
17	Kazmierczak, Magdalena	Machine learning potentials for accurate and efficient multiscale enzymatic Diels – Alder reaction modelling
18	Lei, Li	Coarse-grained investigation of the adsorption behaviour of antibodies at water–hexadecane interfaces
19	Liu, Yufeng	Prediction of rhamnolipid partitioning into lipid bilayers using coarse-grained molecular dynamics with the Martini 3 force field
20	Meadows, James	Controlling Polymorph Crystallisation Using Structured Ternary Fluids
21	Meulemans, Arne	Organic Thermoelectric Polymers: atomistic modelling of semicrystalline P3HT
22	Morado, Joao	Enhancing Electrostatic Embedding for ML/MM Free Energy Simulations
23	Morgan, Liam	Understanding the Behaviour of Hole States for Copper Substitutionals in MgO
24	Novi Inverardi, Giovanni	Structural and dynamical assessment of the adsorption of silica oligomers on biomolecules via Molecular Dynamics
25	Ramos, Carlos	Capturing complexity in enzyme catalysis: Multidimensional Free Energy Landscape Explorations Using Multiscale Methods to Fight Infection Diseases.
26	Sahnoune, Meriem	Coarse-grained modeling of insulin adsorption on plasticized polyvinyl chloride surfaces
27	Thomas, Dominic	Understanding electrochemical interfaces with neural functional theory
28	Tomlinson, Emma	Understanding DNA-Protein Interactions in Eukaryotic Topoisomerases through atomistic molecular
29	Underhill, Juno	Spectral tuning in a de novo riboflavin protein

30	Yang, Chao-Yu	FibrilGen: a program to template cross-β nanostructures at the atomic level
31	Ymeraj, Matilda	Structure-based virtual screening targeting APSR: exploring covalent inhibitors against Pseudomonas
32	Zhang, Xibei	Transforming Tuberculosis Care: Rapid Accurate and Reliable Computer-Based Prediction of Drug Resistance to Guide Targeted Treatments
33	Zhou, Fulu	Applicability of the Thermodynamic and Mechanical Route to the Young Equation for Rigid and Soft Solids: A Molecular Dynamics Simulations Study of a Lennard-Jones System Model
34	Donadoni, Edoardo	Characterizing graphene biointeractions: coarse-grained modeling of ion binding, small molecule adsorption and protein corona formation
35	Güven, Jasmin	Protocols for free energy predictions for beta-lactamases: insights from cross-class inhibitors
36	Kearney, Eoin	Coarse-grained molecular dynamics simulations of surfactant membrane-water partitioning
37	Kolli, Hima Bindu	Multiscale Simulation Scattering Intensity Calculator (MuSSIC):Validation and Application to Soft-Matter Systems
38	Petho, Andras	Investigating the conductivity of multi-heme cytochromes