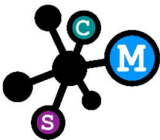


CMS 2024

Time	Wednesday		Thursday		Friday	
	FAB0.03	FAB0.08	FAB0.03	FAB0.08	FAB0.03	FAB0.08
9-10			Keynote talk (FAB0.03) Noa Marom		Keynote talk (FAB0.03) Marjolein Dijkstra	
10-11			Break		Break	
			Contributed talk Edgar Olehnovics	Contributed talk Roya Ebrahimi Vliand	Contributed talk Federico Hernandez	Contributed talk Florian Dietrich
		Contributed talk Roel van de Ven	Contributed talk James Middleton	Invited talk: Tom Penfold	Invited talk Joe Greener	
		Coffee break		Coffee break		
11-12	Registration		Invited talk Carla de Tomas	Invited talk Karen Johnston	Contributed talk Hugh Burton	Contributed talk Fabienne Bachtiger
		Contributed talk Vincent Fletcher	Contributed talk George Marchant	Invited talk David Wilkins	Invited talk Flor Siperstein	
12-13	Lunch (Rootes Restaurant)		Lunch (Rootes Restaurant)		Lunch (Rootes Restaurant)	
13-14	Welcome		Keynote talk (FAB0.03) Sarah Harris		Keynote talk (FAB0.03) Michele Ceriotti	
14-15	Break		Break		RSC Graduate Student Meeting	
	Invited talk Daniel Cole	Invited talk Rachel Crespo-Otero	Invited talk Grant Hill	Invited talk Clotilde Cucinotta		
	Contributed talk Hesam Makki	Contributed talk Tim Hele	Contributed talk Hatem Helal	Contributed talk Zsuzsanna Koczor-Benda		
15-16	Contributed talk Elliot Chan	Contributed talk Dmitry Makhov	Contributed talk Kit Joll	Contributed talk Natalia Martsinovich		
	Coffee break		Coffee break			
16-17	Invited talk Antonia Mey	Invited talk Ralf Tonner-Zech	Keynote talk (FAB0.03) Karsten Reuter			
	Contributed talk Kakali Sen	Contributed talk Lukas Hörmann	Break			
17-18	Contributed talk Matteo Degiacomi	Contributed talk A. Muthuperiyanyagam	Early Career Networking event			
	Contributed talk J. Gonçalves de Abrantes	Contributed talk Akash Hiregange				
18-19	Poster Session & Buffet Dinner/Drinks (Panorama Suite, Rootes Building)					
19-21			Dinner (Rootes Restaurant)			

Wednesday

12.00	Lunch	
13:20	Welcome	
13:30	Multiscale Simulations of Biomolecular Motors (Sarah Harris)	
14:20	Break	
14:30	DE-FF and MACE-OFF: Data-driven interatomic potentials for molecular simulations (Daniel Cole)	Modelling Excited State Processes in Molecular Crystals (Rachel Crespo-Otero)
15:00	Digital Discovery of Semiconducting Polymers: from Chemical Drawing to Electronic Properties (Hesam Makki)	Designer lighting: a radical approach to improving organic light-emitting diodes (Tim Hele)
15:20	Electrostatic embedding of machine learned potentials for accurate and efficient simulation of enzyme catalysis (Elliot Chan)	Ab initio molecular dynamics modelling of the dissociation of hydrofluorocarbon molecules after electron impact in plasma (Dmitry Makhov)
15.40	Coffee Break	
16:10	Can we learn 'the best' Markov Model? (Antonia Mey)	Learning from fundamental surface science for atomic layer deposition – an ab initio endeavour (Ralf Tonner-Zech)
16:40	Combined experimental and computational approaches to characterising the active site structure of cytochrome P460 (Kakali Sen)	Atomic-scale insights into frictional energy dissipation mechanisms (Lukas Hörmann)
17:00	The effect of hydration and dynamics on the mass density of single proteins (Matteo Degiacomi)	The impact of Cu amorphous structure on CO2 electrocatalysis: A combined machine learning and DFT modelling approach (Akshayini Muthuperiyanyagam)
17:20	Tunnelling in methylated DNA using NEO-DFT (Juliana Gonçalves de Abrantes)	Computational Insights into the Stability and Phase Transition of Cobalt Oxide Nanoparticles for Fischer-Tropsch Catalysis (Akash Hiregange)
18.00	Poster session and buffet Dinner	

Thursday

09:00	Computational Discovery of New Materials for Singlet Fission in the Solid State (Noa Marom)	
09:50	Break	
10:00	Assessing the accuracy and efficiency of lattice free energy differences obtained from reweighted flow-based probabilistic generative models (Edgar Olehnovics)	Charge transport simulation using kinetic Monte Carlo with fast update rules (Roya Ebrahimi Viand)
10:20	Finding a needle in a needle stack: Leveraging vibrational spectra and machine learning to guide conformational search (Roel van de Ven)	Exploring Triboelectric Charging Mechanisms with Density Functional Theory (James Middleton)
10:40	Coffee Break	
11:10	Accelerating the prediction of large carbon clusters combining structure search and machine-learning interatomic potentials (Carla de Tomas)	Probing Structural Subtleties in Anti-Perovskite Solid Electrolytes (Karen Johnston)
11:40	Thermodynamically Informed Phase Space Exploration for Optimal Autonomous MLIP Dataset Building (Vincent Fletcher)	Determining phase transitions in magnetic materials from first principles: Case study of MnAl (George Marchant)
12:00	Lunch	
13:30	More than physics, more than data: integrated machine-learning models for materials (Michele Ceriotti)	
14:20	Break	
14:30	Machine learning of Gaussian basis sets for use in molecular applications (Grant Hill)	Exploring the Pt(111)-Electrolyte Interface Under Applied Potentials with Ab Initio Molecular Dynamics (Clotilde Cucinotta)
15:00	MESS: Modern Electronic Structure Simulations (Hatem Helal)	Ab-initio simulation of electron transfer processes of adsorbate-surface systems with ground-state density functional theory (Zsuzsanna Koczor-Benda)
15:20	Machine learning the electric field response of condensed phase systems using perturbed neural network potentials (Kit Joll)	Computational modelling of oxygen-functionalized graphene: structure-property relationship and application in phosphate sensing (Natalia Martsinovich)
15:40	Coffee Break	
16:10	Beyond Crystallinity and Throughput: Machine Learning Accelerated Materials Discovery for Energy Conversion and Storage (Karsten Reuter)	
17:00	Break	
17:10	Early Career Networking Event	
19:00	Dinner	

Friday

09:00	Accelerating the design of Soft Materials using Machine Learning (Marjolein Dijkstra)	
09:50	Break	
10:00	Atomistic photodynamics simulations for solid-state energy materials (Federico Hernandez)	Machine Learning Order Parameters in Atomistic Systems (Florian Dietrich)
10:20	Predicting and Interpreting Femtosecond X-ray spectroscopy (Tom Penfold)	Reversible simulation to train classical and machine learning potentials (Joe Greener)
10:50	Coffee Break	
10:20	Mapping the landscape of electronic structure theory (Hugh Burton)	Efficient calculation of nucleation rates from equilibrium molecular dynamics and a state correspondence principle (Fabienne Bachtiger)
10:40	Surface-Specific Spectroscopy through Machine Learning (David Wilkins)	Coatings for Corrosion Protection: Insights from Molecular Simulations (Flor Siperstein)
12:10	Closing Remarks & Lunch	

