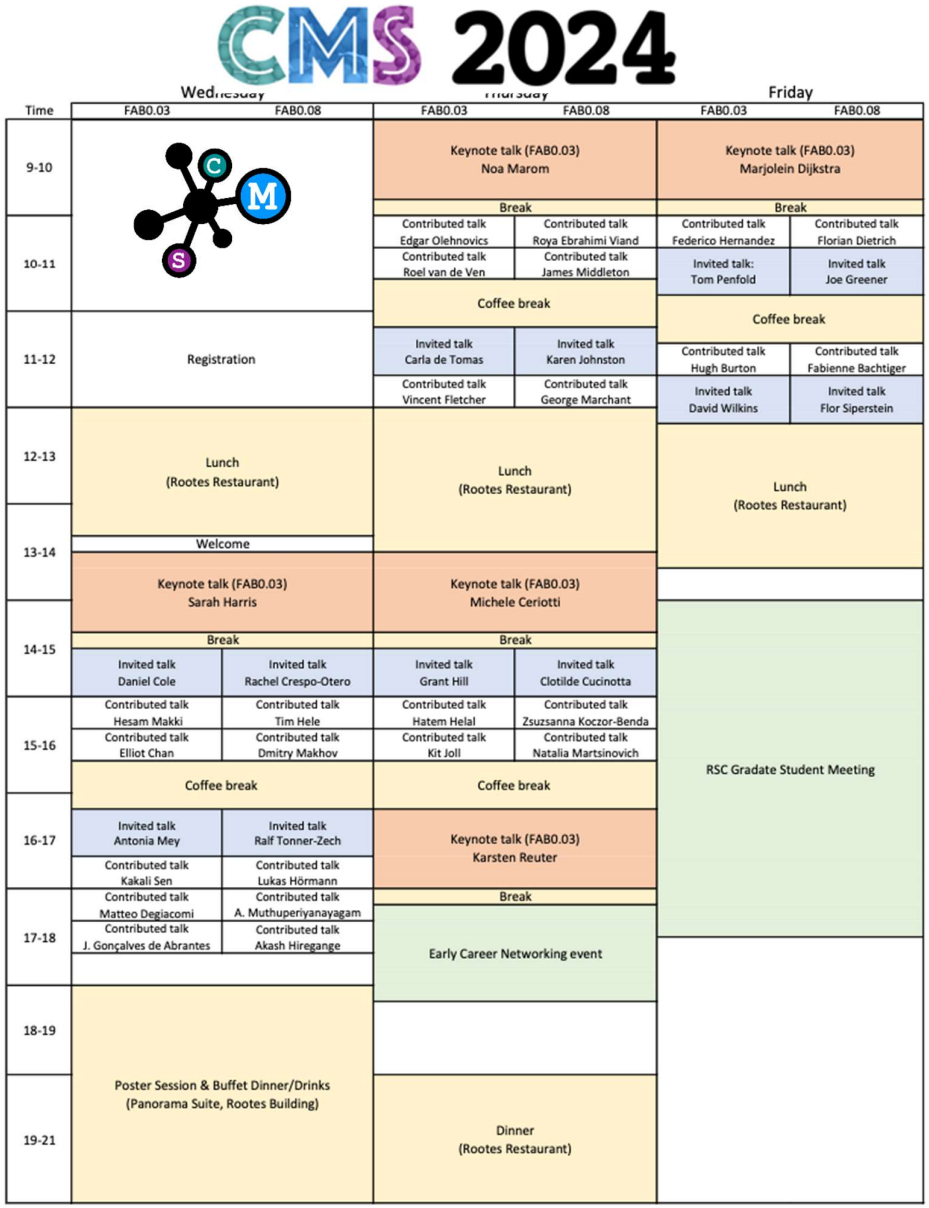
Computational Molecular Science 2024



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 Muthuperiyanayagam)***
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*	

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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*