Wednesday, 6 May

13:00-14:00:	**Registration**	*Foyer*
14:00-14:15:	**Opening & Welcome: Rebecca Wade**	*Carl Bosch Auditorium*
14:15-15:45:	**Session 1 – Chair: Tristan Bereau**	
14:15-14:55:	**Session 1/Talk 1 – Alex Tkatchenko:** *"Machine-Learned Force Fields for Molecular Simulations Beyond AlphaFold and Empirical Potentials"*	
14:55-15:15:	**Session 1/Short talk: Torben Berndt:** *"Approximate Equivariance via Projection-Based Regularisation"*	
15:15-15:35:	**Session 1/Short talk: Van-Quan Vuong:** *"Complete-Basis-Set Extrapolation: What Scheme Is the Best?"*	
15:45-16:30:	*Coffee break*	*Foyer*
16:30-18:10:	**Session 2 – Chair: Rebecca Wade**	*Carl Bosch Auditorium*
16:30-17:10:	**Session 2/Talk 1 – Bingqing Cheng:** *"Energy and forces are all you need"*	
17:10-17:50:	**Session 2/Talk 2 – Qiang Cui:** *"Recent developments and applications of QM/MM-ML free energy methods"*	
17:50-18:10:	**Session 2/Short talk: Cesar Mendoza Martinez:** *"Generation of open states for ion channels using AlphaFold subsampling and intrinsic protein properties"*	

Thursday, 7 May

09:00-10:40:	**Session 3 – Chair: Pascal Friederich**	*Carl Bosch Auditorium*
09:00-09:40:	**Session 3/Talk 1 – Fernanda Duarte:** *"Modelling condensed-phase reactivity with MLIPs"*	
09:40-10:20:	**Session 3/Talk 2 – Luca Ghiringhelli:** *"Learning parsimonious models for materials characterization and design"*	
10:20-10:40:	**Session 3/Short talk: Niccolo Di Eugenio:** *"Machine-Learned Interatomic Potentials for Radiation Damage Analysis in High-Temperature Superconductors"*	
10:40-11:20:	*Coffee break*	*Foyer*
11:20-13:00:	**Session 4 – Chair: Frauke Graeter**	*Carl Bosch Auditorium*
11:20-12:00:	**Session 4/Talk 1 – Patrick Bryant:** *"Beyond the Canonical Alphabet: De Novo Design of Functional Peptides and GPCR Agonists"*	
12:00-12:20:	**Session 4/Short Talk: Chris John:** *"Machine-Learning Framework for Excitation Energies of Chromophores in Polarizable Environments"*	
12:20-13:00:	**Discussion Session – Chair: Fred Hamprecht**	
13:00-14:20:	**Lunch**	*Foyer*
14:20-14:30:	**Group Photo**	*Foyer*

Thursday, 7 May

14:30-16:10:	**Session 5 – Chair: Jan Stuehmer**	*Carl Bosch Auditorium*
14:30-15:10:	**Session 5/Talk 1 – Alexander Tong:** *"Controlling Generative Models"*	
15:10-15:50:	**Session 5/Talk 2 – Ben Murrell:** *"Branching Flows: Discrete, Continuous, and Manifold Flow Matching with Splits and Deletions"*	
15:50-16:10:	**Session 5/Short Talk – Riccardo Beccaria:** *"Physics Informed Machine Learning Potential for Brownian Dynamics Simulations"*	
16:10-16:40:	*Coffee break*	*Foyer*
16:40-18:00:	**Session 6 – Chair: Alice Allen**	*Carl Bosch Auditorium*
16:40-17:20:	**Session 6/Talk 1 – Yair Litman:** *"Molecular Strategies for Confinement-Controlled Water Structure and Chemistry"*	
17:20-17:40:	**Session 6/Short talk – Roman Remme:** "Surrogate Functionals for Machine-Learned Orbital-Free Density Functional Theory"	
17:45-19:00:	**Poster session**	*Foyer*
19:00-22:00:	**Scientist evening session with finger food + Poster session (Studio)**	

Friday, 8 May

09:00-10:40:	**Session 7 – Chair: Fred Hamprecht**	*Carl Bosch Auditorium*
09:00-09:40:	**Session 7/Talk 1 – Ilyes Batatia:** *"Foundational Machine Learning Force Fields for Atomistic Chemistry"*	
09:40-10:20:	**Session 7/Talk 2 – Pratyush Tiwary:** *"Efficient, explainable and extrapolative AI for biophysics"*	
10:20-10:40:	**Session 7/Short talk: Tobias Kaczun:** *"Taking the next Step with Machine Learning Orbital Free DFT"*	
10:40-11:10:	*Coffee break*	*Foyer*
11:10-12:10:	**Session 8 – Chair: Alice Allen**	*Carl Bosch Auditorium*
11:10-11:50:	**Session 8/Talk 1 – Martin Stoehr:** "Differentiable Quantum Chemistry: Hybrid Machine Learning Models and More"	
11:50-12:10:	**Session 8/Short talk: Henrik Christiansen:** *"Hyperspatial Sampling"*	
12:10-13:00:	**Roundup**	
13:00-14:30:	**Lunch & End of Workshop**	*Foyer*