Wednesday, 7 May

13:00-14:00:	**Registration**	*Foyer*
14:00-14:15:	**Opening & Welcome: Rebecca Wade & Kai Polsterer**	*Carl Bosch Auditorium*
14:15-15:45:	**Session 1 – Chair: Rebecca Wade**	
14:15-14:55:	**Session 1/Talk 1 – Modesto Orozco:** *"Nucleic acids in the frontier between AI and simulation"*	
14:55-15:15:	**Session 1/Short talk: Patrizia Mazzeo:** *"Excited-state dynamics of solvated molecules with multiscale machine learning"*	
15:15-15:35:	**Session 1/Short talk: Abhik Ghosh Moulick** *"Towards Understanding of Chromatin Folding: The Role of Protein Interactions for Stability of Nucleosomes"*	
15:45-16:30:	*Coffee break*	*Foyer*
16:30-18:10:	**Session 2 – Chair: Ullrich Köthe**	*Carl Bosch Auditorium*
16:30-17:10:	**Session 2/Talk 1 – Carolin Müller:** *"Machine Learning in Photochemistry – Data is Key"*	
17:10-17:50:	**Session 2/Talk 2 – Johannes Kästner:** *"Transferable and Uniformly Accurate Interatomic Potentials"*	
17:50-18:10:	**Session 2/Short talk: – Leif Seute:** *"Learning conformational ensembles of proteins based on backbone geometry"*	

Thursday, 8 May

09:00-10:40:	**Session 3 – Chair: Frauke Gräter**	*Carl Bosch Auditorium*
09:00-09:40:	**Session 3/Talk 1 – Arne Elofsson:** *"Towards a Complete Structural Map of the Human Proteome Using AlphaFold"*	
09:40-10:20:	**Session 3/Talk 2 – Matteo dal Peraro:** *"A Structure Transformer for Structural Biology and Molecular Design"*	
10:20-10:40:	**Session 3/Short talk: Sergio Suarez Dou** *"Machine Learning Force Field modelling for quantum accuracy in biomolecule dynamics"*	
10:40-11:20:	*Coffee break*	*Foyer*
11:20-13:00:	**Session 4 – Chair: Alice Allen**	*Carl Bosch Auditorium*
11:20-12:00:	**Session 4/Talk 1 – Stefan Grimme:** *"g-xTB: DFT accuracy at tight-binding speed"*	
12:00-12:20:	**Session 4/Short Talk: Oleksandra Kukharenko** *"Utilizing generative machine learning models to improve determinination of glass transition in polymer melts"*	
12:20-13:00:	**Discussion Session – Chair: Alice Allen**	
13:00-14:20:	**Lunch**	*Foyer*
14:20-14:30:	**Group Photo**	*Foyer*

Thursday, 8 May

14:30-16:10:	**Session 5 – Chair: Marcus Elstner**	*Carl Bosch Auditorium*
14:30-15:10:	**Session 5/Talk 1 – Shirin Faraji:** *"On-the-fly hybrid quantum/classical dynamics in complex environment"*	
15:10-15:50:	**Session 5/Talk 2 – Sandra Luber:** *"Excited states dynamics and beyond"*	
15:50-16:10:	**Session 5/Short Talk: Henrik Schopmans** *"Temperature-Annealed Boltzmann Generators"*	
16:10-16:40:	*Coffee break*	*Foyer*
16:40-18:00:	**Session 6 – Chair: Andreas Dreuw**	*Carl Bosch Auditorium*
16:40-17:20:	**Session 6/Talk 1 – Marc van der Kamp:** *"EMLE: Electrostatic Machine-Learned Embedding for accurate and efficient ML/MM simulations of enzymes and other biomolecules"*	
17:20-17:40:	**Session 6/Short talk – Sarah Bernart:** *"Machine Learning-Driven Insights into Active Species and Reaction Dynamics in Pd and Pt Catalysts Supported on Ceria"*	
17:45-19:00:	**Poster session**	
19:00-22:00:	**Workshop Dinner + Poster session (Studio)**	*Foyer*

Friday, 9 May

09:00-10:40:	**Session 7 – Chair: Tristan Bereau**	*Carl Bosch Auditorium*
09:00-09:40:	**Session 7/Talk 1 – Lukas Stelzl:** *"Dynamic self organization of proteins in the cell nucleus"*	
09:40-10:20:	**Session 7/Talk 2 – Elsa Sánchez-García** *"Combining Machine-Learning and Physics-Based Approaches for Computer-Aided Drug Design and Protein Engineering"*	
10:20-10:40:	**Session 7/Short talk: Fabian Grünewald** *"From CGsmiles to multiresolution GNNs for chemical space exploration"*	
10:40-11:10:	*Coffee break*	*Foyer*
11:10-12:10:	**Session 8 – Chair: Pascal Friederich**	*Carl Bosch Auditorium*
11:10-11:50:	**Session 8/Talk 1 – Antonia Mey:** *"From generative modelling for fragment-based drug design to property prediction based on large-language models"*	
11:50-12:10:	**Session 8/Short talk: Luis Walter** *"Navigating Chemical Space: An Active Learning Strategy Using Multi-Level Coarse-Graining"*	
12:10-13:00:	**Roundtable Discussion & Roundup – Chairs: Anya Gryn'ova; Tristan Bereau**	
13:00-14:30:	**Lunch & End of Workshop**	*Foyer*