

Wednesday, 7 May

13:00-14:00:	Registration	Foyer
14:00-14:15:	Opening & Welcome: Rebecca Wade & Kai Polsterer (HITS)	Carl Bosch Auditorium
14:15-15:45:	Session 1 – Chair: Rebecca Wade	
14:15-14:55:	Session 1/Talk 1 – Modesto Orozco: <i>"Nucleic acids in the frontier between AI and simulation"</i>	
14:55-15:15:	Session 1/Short talk: Patrizia Mazzeo: <i>"Excited-state dynamics of solvated molecules with multiscale machine learning"</i>	
15:15-15:35:	Session 1/Short talk: Abhik Ghosh Moulick <i>"Towards Understanding of Chromatin Folding: The Role of Protein Interactions for Stability of Nucleosomes"</i>	
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: <i>"Machine Learning in Photochemistry – Data is Key"</i>	
17:10-17:50:	Session 2/Talk 2 – Johannes Kästner: <i>"Transferable and Uniformly Accurate Interatomic Potentials"</i>	
17:50-18:10:	Session 2/Short talk: Hamza Siddiqui <i>"Interpretable AI and Machine Learning Classification for Identifying High-Efficiency Donor–Acceptor Pairs in Organic Solar Cells"</i>	

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

Thursday, 8 May

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

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