Wednesday May 15, 2024			
Registration	13:00		
Opening	14:00	Rebecca Wade, Tilmann Gneiting	
Session 1			
Session Chair		Frauke Gräter	
Talk 1	14:15	Sandra Luber	Excited state dynamics and beyond
Talk 2	14:55	Mark E. Tuckerman	Synergizing enhanced sampling and machine learning strategies in molecular simulation for representing and deploying high-dimensional free energy surfaces and learning reaction coordinates
Short presentation	15:40	Andres Escorcia	Multi-scale simulations reveal a Cys-His-Water-Glu catalytic network in Cezanne-2
Coffee break	16:00		
Session 2			
Session Chair		Tristan Bereau	
Talk 1	16:30	Matteo Degiacomi	Learning (from) protein dynamics
Talk 2	17:10	Roberto Covino	Molecular Free Energies, Rates, and Mechanisms from Machine learning-guided Path Sampling Simulations
Short presentation	17:50	Aleksander Durumeric	Coarse-grained molecular dynamics for proteins with neural networks: Challenges and breakthroughs
Photo speaker			
Invited speakers' dinner	19:00		

Thursday May 16, 2024			
Session 3			
Session Chair		Pascal Friederich	
Talk 1	09:00	Johannes Margraf	Science-Driven Chemical Machine Learning
Talk 2	09:40	Geemi Wellawatte	Explainable AI in Chemistry
Short Talk	10:20	Luis Itza Vazquez Salazar	Asparagus: a toolkit for automatic construction of machine-learned potential energy surfaces
Coffee break	10:40		
Session 4			
Session Chair		Marcus Elstner	
Talk 1	11:20	Lorenzo Cupellini	Understanding electronic excitations in complex systems with machine learning
Short Talk	12:00	Daniel Bultrini	Mixed quantum-classical dynamics for near term quantum computers
Discussion round table	12:20		Chairs: Pascal Friederich, Fred Hamprecht
Lunch	13:00		
Photo all	14:20		
Session 5			
Session Chair		Rebecca Wade	
Talk 1	14:30	Felice Lightstone	Using the Multiscale Machine-Learned Modeling Infrastructure (MuMMI) to Explore Protein Conformational Paths for RAS-RAF Activation
Talk 2	15:10	Edina Rosta	Enhanced Sampling Simulations of Biomolecular Systems
Short Talk	15:50	Ludovico Pupito	Molecular Pathways unveiled by with Multiple Walker Supervised Molecular Dynamics
Coffee break	16:10		
Session 6			
Session Chair		Ullrich Köthe	
Talk 1	16:40	Julia Westermayr	Advancing excited-state simulations with machine learning
Talk 2	17:20	Grant Rotskoff	Accelerating Biomolecular Ensemble Sampling with Generative Neural Networks
Short Talk	18:00	Stiv Llenga	Spying On Molecules: Constructing Novel Compound Spaces via Molecular Triangulation
Poster session	18:20		
Workshop Dinner + Poster	19:00		

Friday May 17, 2024			
Session 7			
Session Chair		Fred Hamprecht	
Talk 1	09:00	Boris Kozinsky	Combining data, physics and machine learning for accelerating materials computations
Talk 2	09:40	Andrea Volkamer	Hybrid AI for Molecular Design
Short Talk	10:20	Leif Seute	Learning a State of the Art MM Force Field
Coffee break	10:40		
Session 8			
Session Chair		Anya Grynova	
Talk 1	11:20	Alessandro Troisi	Digital Discovery of Organic Electronics Materials
Short Talk	12:00	Anita Ragyanszki	Understanding the Origins of Life - A Machine learning approach to estimate reaction mechanisms of biotic precursors
Discussion round table and round up	12:20		Chairs: Rebecca Wade, Rostislav Fedorov
Lunch	13:00		
End	14:30		
IBM Software Workshop ?			