Sunday (March 9th)		
18:00	Dinner @ la Posta de Mesilla	
Monday Morning (March 10th)		
7:50	**Greg Voth, Chicago**	Opening Remarks
8:00	**Hua Guo, New Mexico**	Machine learning approaches to solving the Schrodinger equation
8:30	**Tim Berkelbach, Columbia University**	Quantum chemistry and machine learning
9:00	**Rui Sun, Hawaii**	Great power comes with great risk - ML potential in reaction dynamics simulations
9:30	**Toshiyuki Takayanagi, Saitama University**	Application of machine-learning techniques to reaction dynamics studies
10:00	--------- Break ---------	
10:30	**Greg Voth, Chicago**	Machine learning and ultra-coarse-graining
11:00	**Grant Rotskoff, Stanford**	Accelerating generative conformational search with energy rank alignment
11:30	**Wanlu Li, USCD**	Structural prediction of high-entropy materials
12:00	**Xiaorong Liu, New Mexico**	Enhanced sampling in high-throughput free energy calculations
12:30	--------- Morning Session Adjourned ---------	
Tuesday Morning (March 11th)		
8:00	**Chris Chipot, CERN**	Machine learning approaches for modeling rare events: towards unveiling conformational transitions in biological objects
8:30	**Margaret Johnson, Johns Hopkins University**	Learning optimal self-assembly kinetics using automatic differentiation
9:00	**Omar Valsson, North Texas**	Unraveling protein-protein dissociation kinetics via atomistic simulations and machine learning methods
9:30	**Xuhui Huang, Wisconsin**	Discovering slow collective variables of biomolecular dynamics by minimizing time integrations of memory kernels via neural networks
10:00	--------- Break ---------	
10:30	**Suriyanarayanan Vaikuntanathan, Chicago**	Generative diffusion with active dynamics
11:00	**Glen Hocky, NYU**	Good rates from bad coordinates
11:30	**David Limmer, Berkerly**	Deep learning the reaction path ensemble
12:00	--------- Morning Session Adjourned ---------	
Tuesday Afternoon (March 12th)		
14:00	**Rafael Gomez-Bombarelli, MIT**	ML gradients in molecular simulations: from force fields to alchemy
14:30	**Markus Meuwly, University of Basel**	Machine learning inter- and intramolecular interactions for chemical reaction dynamics
15:00	**Habib N Najm, Sandia NL**	Machine learning reactive potential energy surfaces for hydrocarbon molecules

15:30	**Zhou Lin, UMass**	Integrating graph neural networks and density functional theory in many-body expansion theory for high-dimensional potential energy surfaces
16:00	--------- Break ---------	
16:30	**Yi He, New Mexico**	Leveraging generative AI for constructing intrinsically disordered protein ensembles from chemical shift data
17:00	**Alex Pak, Colorado Mines**	Probabilistic forecasting for coarse-grained molecular dynamics
17:30	**Yihang Wang, Chicago**	Towards kinetic accuracy in coarse-grained models with machine learning
18:00	--------- Afternoon Session Adjourned ---------	
	Wednesday Morning (March 12th)	
8:00	**Ed Maginn, Notre Dame**	Sustainable Materials Discovery Via Machine Learning Enabled Molecular Simulations
8:30	**Bingqing Cheng, Berkeley**	Cartesian atomic cluster expansion for machine learning potentials
9:00	**Todd Gingrich, Northwestern**	Learning to build a molecular motor
9:30	**Simon Olsson, Chalmers**	Generative AI for Multi-scale Simulation
10:00	--------- Break ---------	
10:30	**Ming Chen, Purdue**	Generating Protein Conformational Ensemble: Enhanced Sampling, Coarse-grained Model, and Machine Learning
11:00	**Upakarasamy Lourderaj, NISER**	ML representation of potential energy surfaces for reaction dynamics simulations
11:30	**Yinan Shu, Minnesota**	Advances in Coupled Potential Energy Surfaces Learning for Nonadiabatic Dynamics
12:00	--------- Meeting Adjourned ---------	