

**Molecular Simulation with Machine Learning**  
**Workshop Program**  
*Eastern Standard Time (EST)*

<b>Monday, July 13th</b>		
<b>Time</b>	<b>Speaker</b>	<b>Title</b>
<i>Morning session 1, chair: Tom Gartner (Princeton U.)</i>		
9:00 - 9:30am	<b>Weinan E (Princeton U.)</b>	Machine learning assisted modeling
9:30 - 10:00am	<b>Roberto Car (Princeton U.)</b>	Molecular simulation with the deep potential method
10:00 - 10:30am	<b>Pablo Piaggi (Princeton U.)</b>	The art of non-Boltzmann sampling
10:30 - 11:00am	<i>Breakout session</i>	
<i>Morning session 2, chair: Amartya Bose (Princeton U.)</i>		
11:00 - 11:30am	<b>Gary Grest (LANL)</b>	Introduction to LAMMPS Molecular Dynamics Simulator
11:30 - 12:00pm	<b>Thomas Kuhne (U. of Paderborn)</b>	CP2K/Quickstep: The Swiss Army Knife of Molecular Simulation
12:00 - 12:30pm	<b>Menno Bokdam (U. of Vienna)</b>	Entropy-driven phase transformations in hybrid perovskites simulated by on-the-fly machine-learning force fields
<i>Tutorial session 1, hosts: Marcos Calegari-Andrade, Yixiao Chen, Tom Gartner, Pablo Piaggi, Shuwen Yue, Linfeng Zhang</i>		
14:00 - 17:30pm	<i>Tutorial example 1</i>	

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<b>Tuesday, July 14th</b>		
<b>Time</b>	<b>Speaker</b>	<b>Title</b>
<b>Morning session 3, chair: Pablo Piaggi (Princeton U.)</b>		
9:00 - 9:30am	<b>Michele Ceriotti (EPFL)</b>	Equivariant representations for atomistic machine learning
9:30 - 10:00am	<b>Sebastian Dick (SUNY)</b>	Machine learned XC potentials in Siesta: NeuralXC
10:00 - 10:30am	<b>Davide Tisi (SISSA)</b>	Green Kubo simulation of transport properties from ab initio to neural networks
10:30 - 11:00am	<b>Breakout session</b>	
<b>Morning session 4, chair: Zachary Goldsmith (Princeton U.)</b>		
11:00 - 11:30am	<b>Robert A. DiStasio (Cornell U.)</b>	DFT and Beyond: Benchmark Data for Next-Generation Machine Learning of Intra- and Inter-Molecular Interactions
11:30 - 12:00pm	<b>J. Mark Martirez (UCLA)</b>	Density-functional-theory-based embedding theories for embedded correlated wavefunction description of molecules and surfaces
12:00 - 12:40pm	<b>Round table discussion. Panelists: All the speakers plus Stefano Baroni (SISSA), Paolo Giannozzi (U. Udine), L. Zhang</b>	
<b>Tutorial session 1, hosts: Marcos Calegari-Andrade, Yixiao Chen, Tom Gartner, Pablo Piaggi, Shuwen Yue, Linfeng Zhang</b>		
14:00 - 17:30pm	<b>Tutorial example 2</b>	