	Monday, Sep 10	**Tuesday**, Sep 11	**Wednesday**, Sep 12	**Thursday**, Sep 13	**Friday**, Sep 14
09:00	opening	**Learning effective molecular models from experimental observables** Cecilia Clementi (Rice)	**High Dimensional Neural Network Potentials** Jörg Behler (U Göttingen)	**Workshop 1** Marc Mosch Josua Vieten	**Workshop 4** Nicola Marzari
09:30	**Image processing and supervised/unsupervised machine learning** Roger French (Case Western)				
10:00					*coffee break*
10:30		*coffee break*	*coffee break*	*coffee break*	**Workshop 5** Roger French
11:00	*coffee break*	**Machine Learning for Synthetic Chemistry** Connor Coley (MIT)	**Concepts, Challenges, and Results of the NOMAD Laboratory** Pasquale Pavone (HU Berlin)	**Workshop 2** Kristian Thygesen Daniel Urban Peter Steinbach	
11:30	**Introduction to Machine Learning with Python** Thomas Lehmann (TU Dresden)				*luncheon*
12:00					
12:30		*luncheon*	*luncheon*		
13:00	*luncheon*			*luncheon*	Round Table with Participants
13:30					
14:00	**Introduction to Graph-based Learning** Dominik Alfke (TU Chemnitz)	**Machine Learning for Molecular Dynamics** Frank Noe (FU Berlin)	**High-throughput computational discovery of novel opto-electronic materials** Kristian Thygesen (DTU)	**Workshop 3** Jörg Schuster Reinhard Scholz S. Mehdi Vaez Allaei	
14:30					
15:00					closing
15:30	*coffee break*	*coffee break*	*coffee break*		
16:00	hands on	hands on	hands on	*coffee break*	
16:30				contributed talks	
17:00	Get-to-Know	Poster Session			
17:30					
18:00					
18:30					
19:00					
19:30					
20:00					

Lectures

Cecilia Clementi	Learning effective molecular models from experimental observables
Connor Coley	Machine Learning for Synthetic Chemistry
Dominik Alfke	Introduction to Graph-based Learning
Frank Noe	Machine Learning for Molecular Dynamics
Jörg Behler	High Dimensional Neural Network Potentials
Kristian Sommer Thygesen	High-throughput computational discovery of novel opto-electronic materials
Pasquale Pavone	Concepts, Challenges, and Results of the NOMAD (Novel Materials Discovery) Laboratory
Roger French	Computer Vision and Machine Learning in a Distributed Computing Environment: Photovoltaic Degradation Quantified Using Electroluminescent Images
Thomas Lehmann	Introduction to Machine Learning with Python

Workshops

Daniel Urban	A machine-learning approach for the discovery of novel hard-magnetic phases
S. Mehdi Vaez Allaei	Phononic heat transport and thermal rectification in low dimensional heterostructures
Roger French	Time Series Analysis and Network Modeling of PV Modules and Power Plants to Decrease Degradation Rates
Kristian Sommer Thygesen	*High-throughput computational discovery of novel opto-electronic materials II*
Nicola Marzari	Computational design and discovery of novel materials
Josua Vieten	Perovskite Materials design for two-step thermochemical processes
Marc Mosch	The Material HUB
Jörg Schuster	Simulation of Materials, Processes and Devices for Nanoelectronics Engineering
Peter Steinbach	*Benchmarks of and hardware for machine learning*
Reinhard Scholz	Thermally activated delayed fluorescence - A new route to more efficient OLEDs?

Contributed Talks

Nikita Sengar	Bayesian Optimization to Model Polymorphism and Phase Transition Mechanisms in Small Molecule Organic Semiconductors
Antonis Stellas	Smart nanometrology with artificial intelligence
Tuan Nguyen	Design of bio-inspired materials: Emerging innovation from deep learning