

## Workshop III: Collective Variables in Quantum Mechanics

**Monday November 14, 2016**

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–9:50 **Stéphane Mallat** (École Normale Supérieure)  
*Quantum Chemistry Energy Regression and Statistical Physics with Scattering Transforms*
- 10:00–10:15 *Break*
- 10:15–11:05 **Gabor Csányi** (University of Cambridge)  
*Learning quantum potential energy surfaces: multiple descriptors, many body expansions, baselines*
- 11:15–11:30 *Break*
- 11:30–12:20 **Alexandre Tkatchenko** (University of Luxembourg)  
*Collective Variables in Quantum Mechanics and Machine Learning*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Glenn Martyna** (IBM Watson Research Center)  
*An electronically coarse grained model including all quantum mechanical fluctuations necessary for long-range forces describes water's properties from ice to the supercritical regime*
- 3:30–4:00 *Break*
- 4:00–4:50 **Alberto Ambrosetti** (Università degli Studi di Padova)  
*Towards controllable van der Waals interactions: the importance of collective charge dynamics at the nanoscale*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

**Tuesday November 15, 2016**

- 8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Reinhold Schneider** (Technische Universität Berlin)  
*Hierarchical Tensor Approximation, DMRG and Combination with a Multi-Reference Coupled Cluster Method*
- 10:00–10:15 *Break*
- 10:15–11:05 **Yvon Maday** (Université de Paris VII (Denis Diderot) et Université de Paris VI (Pierre et Marie Curie))  
*Combining model reduction methods and data assimilation tools for the approximation of the solution to parameter dependent PDE's : Application to quantum mechanics*
- 11:15–11:30 *Break*

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- 11:30–12:20 **Markus Reiher** (Swiss Federal Institute of Technology of Zurich)  
*Extracting Chemical Information from Quantum Many-Particle Physics*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Olexandr Isayev** (University of North Carolina)  
*Predicting Properties and Electronic Structure of Inorganic Materials with Machine Learning*
- 3:30–4:00 *Break*
- 4:00–4:50 **Kieron Burke** (University of California, Irvine (UCI))  
*DFT and ML: The role of collective variables*

### Wednesday November 16, 2016

- 8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Alexander Shapeev** (Skolkovo Institute of Science and Technology)  
*Toward accurate, efficient, and reliable interatomic potentials*
- 10:00–10:15 *Break*
- 10:15–11:05 **Noa Marom** (Carnegie-Mellon University)  
*Effect of Crystal Packing on the Electronic Properties of Molecular Crystals*
- 11:15–11:30 *Break*
- 11:30–12:20 **Gus Hart** (Brigham Young University)  
*Grain Boundary Physics, Machine Learning, and the SOAP Formalism*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Benjamin Stamm** (RWTH Aachen)  
*Reducing complexity by implicit solvation models.*
- 3:30–4:00 *Break*
- 4:00–4:50 **Lin Lin** (University of California, Berkeley (UC Berkeley))  
*Density functional perturbation theory for large systems*

### Thursday November 17, 2016

- 8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Alessandro De Vita** (King's College London)  
*Inference-Boosted First Principles Molecular Dynamics*
- 10:00–10:15 *Break*

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- 10:15–11:05 **Tristan Bereau** (Max Planck Institute for Polymer Research)  
*Combination of physics-based and data-driven methods to parametrize polarizable intermolecular potentials across small organic molecules*
- 11:15–11:30 *Break*
- 11:30–12:20 **Harald Oberhofer** (Technical University Munich (TUM))  
*Virtual Screening for High Carrier Mobility in Organic Semiconductors*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:55 **Short Presentations**  
*by Stefan Chmiela, Grégoire Ferré and Jan Hermann*
- 4:00–4:15 *Break*
- 4:15–5:00 **Panel Discussion**  
*TBA*

## Friday November 18, 2016

- 8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Gero Friesecke** (Technische Universität München)  
*The density-to-pair-density map in density functional theory*
- 10:00–10:15 *Break*
- 10:15–11:05 **Anastassia Alexandrova** (University of California, Los Angeles (UCLA))  
*Ensemble-Average Representation of Pt clusters in Conditions of Catalysis, accessed through GPU Accelerated Deep Neural Network Fitting Global Optimization*
- 11:15–11:30 *Break*
- 11:30–12:20 **Klaus-Robert Müller** (Technische Universität Berlin)  
*Explaining and Understanding Non-linear Classifier Decisions with Application to Deep Learning*
- 12:30 *Conclusion*

