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 Universtitat 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 Decidions with Application to Deep Learning

12:30 *Conclusion*