Understanding Many-Particle Systems with Machine Learning

Tuesday September 20, 2016

3:30–4:30 **Geneviève Dusson** (Université de Paris VI (Pierre et Marie Curie))
MPS Seminar Series: Estimation for Density Functional Theory

Thursday September 22, 2016

3:30–4:00 **Farren Curtis** (Tulane University)
MPS Seminar: Molecular crystal structure prediction with the GAtor genetic algorithm package

Friday September 23, 2016

11:00–12:00 **Risi Kondor** (University of Chicago)
Kernel Methods Tutorial

Tuesday October 4, 2016

3:30–4:00 **Ralf Banisch** (Freie Universität Berlin)
MPS Seminar: Learning persistent dynamical structures from data with diffusion maps

4:00–4:30 **Li Li and Felix Brockherde**
Machine learning meets DFT: various aspects

Thursday October 6, 2016

3:30–4:00 **Katerine Saleme Ruiz** (George Mason University)
MPS Seminar: A fracture model based on a discrete element method for polycrystalline materials

4:00–4:30 **Kristof Schütt** (Technische Universität Berlin)
Learning Atomistic Representations with Deep Tensor Neural Networks

Tuesday October 11, 2016

3:30–4:00 **Marina Meila** (University of Washington)
MPS Seminar: Manifold Learning Tutorial

Thursday October 13, 2016

3:30–4:00 **Chris Anderson** (University of California, Los Angeles (UCLA))
MPS Seminar: Construction of Ab-Initio methods using grid based discretizations

Tuesday October 18, 2016

3:30–4:00 **Alexander Shapeev** (Skolkovo Institute of Science and Technology)
MPS Seminar: Active learning of linear interatomic potentials

4:00–4:30 **Lorenzo Boninsegna** (Rice University)
Complex energy landscapes: Theory and applications

Thursday October 20, 2016

3:30–4:00 **Grégoire Ferré** (École Nationale des Ponts-et-Chaussées (ENPC))
Learning potential energy landscapes with localized graph kernels

Tuesday November 1, 2016

3:30–4:00 **Glenn Martyna** (IBM Thomas J. Watson Research Center)
The Piezoelectronic Transistor - A nanoscale, strain-based transduction device for fast low power switching

4:00–4:30
TBA

Thursday November 3, 2016

3:30–4:00 **Martin Stöhr** (Technical University Munich (TUM))
c-vdW: A charge population analysis-based approach to dispersion interactions

4:00–4:30
TBA

Tuesday November 8, 2016

3:30–4:00 **Ying Li** (Argonne National Laboratory)
MPS Seminar: Nanocarbon Synthesis by High-temperature Oxidation of Nanoparticles

4:00–4:30 **Johannes Hoja** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
First-Principles Modeling of Molecular Crystals: The Role of Collective van der Waals Interactions and Thermal Fluctuations

Wednesday November 9, 2016

3:30–4:00 **Risi Kondor** (University of Chicago)
Low rank and multiresolution approaches to accelerating kernel machines

Thursday November 10, 2016

11:00–11:30 **Alexandre Tkatchenko** (University of Luxembourg)
A primer on van der Waals interactions and quantum fluctuations

3:30–4:00 **Jan Hermann** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Nanoscale pi-pi stacked complexes bound by collective charge fluctuations

4:00–4:30 **Sadasivan Shankar** (Harvard University)
Why Molecular Design is so Hard in Practice?

Tuesday November 22, 2016

11:00–12:00 **Alexandre Tkatchenko** (University of Luxembourg)
A primer on van der Waals interactions and quantum fluctuations (Part 2)

Tuesday November 29, 2016

3:30–4:00 **Mojtaba Haghighatlari** (SUNY Buffalo)
From Structural Analysis to Fingerprints for Molecular Property Predictions

Wednesday November 30, 2016

3:30–4:00 **Claudia Draxl** (Humboldt-Universität)
Tutorial: Big data analytics toolkit at NoMad

Thursday December 1, 2016

3:00–3:30 **Farnaz Heidar-Zadeh** (McMaster University)
How Pervasive is the Hirshfeld Partitioning?

3:30–4:00 **Huziel Sauceda** (National Autonomous University of Mexico (UNAM))
Molecular dynamics using accurate energy-conserving machine learned force fields