

## Machine Learning for Many-Particle Systems

Monday February 23, 2015

- 8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:50–9:00 *Welcome and Opening Remarks*
- 9:00–9:40 **Klaus-Robert Müller** (Technische Universität Berlin)  
*Machine Learning Representation for Materials*
- 10:00–10:15 *Break*
- 10:15–10:55 **Gabor Csányi** (University of Cambridge)  
*Machine learning the Born-Oppenheimer potential energy surface: from materials to molecules*
- 11:15–11:30 *Break*
- 11:30–12:10 **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne (EPFL))  
*Finding patterns and drawing maps in the configuration space of materials and molecules*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:40 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Big Data of Materials Science – Critical Role of the Descriptor(\*)*
- 3:00–3:15 *Break*
- 3:15–3:55 **Joachim Buhmann** (ETH Zürich)  
*Information theory of algorithms*
- 4:15–4:30 *Break*
- 4:30–5:10 **Kieron Burke** (University of California, Irvine (UCI))  
*Finding density functionals with machine learning*
- 5:30–7:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday February 24, 2015

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:40 **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Many Particles, Collective Variables, and Machine Learning*
- 10:00–10:15 *Break*

*(Tuesday schedule continued on next page)*



*(Tuesday schedule continued from previous page)*

- 10:15–10:55 **Alán Aspuru-Guzik** (Harvard University)  
*Machine learning applied to organic materials discovery*
- 11:15–11:30 *Break*
- 11:30–12:10 **Veronique Van Speybroeck** (Ghent University)  
*Exploring new frontiers in modeling complex chemical transformations in nanoporous materials*
- 12:30–1:45 *Lunch (on your own)*
- 1:45–2:25 **Gus Hart** (Brigham Young University)  
*High-throughput Data and New representations for Models and Machine Learning*
- 2:45–3:25 **Peter Minary** (University of Oxford)  
*Simulation of biomolecules: a hierarchical approach*
- 3:45–4:15 *Break*
- 4:15–4:55 **Cecilia Clementi** (Rice University)  
*Multiscale characterization of macromolecular dynamics*
- 5:15–5:55 **Sameer Varma** (University of South Florida)  
*Allosteric regulation of Paramyxovirus Entry into Host Cells: Machine learning to the rescue*

### Wednesday February 25, 2015

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:40 **Krishna Rajan** (Iowa State University)  
*Exploring the Topology of Data in Materials Science*
- 10:00–10:15 *Break*
- 10:15–10:55 **Anatole von Lilienfeld** (Argonne National Laboratory)  
*Machine Learning Models in Chemical Space*
- 11:15–11:30 *Break*
- 11:30–12:10 **Johannes Hachmann** (SUNY Buffalo)  
*Molecular properties from Big Data*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:40 **Stéphane Mallat** (École Normale Supérieure)  
*Quantum Chemistry Energy Regression with Deep Scattering Networks*
- 3:00–3:15 *Break*

*(Wednesday schedule continued on next page)*

*(Wednesday schedule continued from previous page)*

- 3:15–3:55     **Matthias Rupp** (Universität Basel)  
*Properties of Atoms in Molecules via Machine Learning*
- 4:15–4:30     *Break*
- 4:30–5:10     **Aidan Thompson** (Sandia National Laboratories)  
*Atomistic Materials Simulation Using Quantum-Accurate Interatomic Potentials*

### Thursday February 26, 2015

- 8:00–9:00     *Continental Breakfast*
- 9:00–9:40     **Michael Stein** (University of Chicago)  
*Theory and Computation for Gaussian Processes*
- 10:00–10:15   *Break*
- 10:15–10:55   **Risi Kondor** (University of Chicago)  
*Multiresolution Matrix Factorization*
- 11:15–11:30   *Break*
- 11:30–12:10   **Francesco Paesani** (University of California, San Diego (UCSD))  
*Many-Body Molecular Dynamics for Chemically Accurate Simulations from the Gas to the Condensed Phase*
- 12:30–2:00    *Lunch (on your own)*
- 2:00–2:40     **Jonathan Weare** (University of Chicago)  
*Stratification of Markov processes for rare event simulation*
- 3:00–3:15     *Break*
- 3:15–3:55     **Danny Neuhauser** (University of California, Los Angeles (UCLA))  
*Stochastic Quantum Chemistry for Giant Systems*
- 4:15–4:30     *Break*
- 4:30–5:10     **Gitta Kutyniok** (Technische Universität Berlin)  
*Applied Harmonic Analysis meets Compressed Sensing*

### Friday February 27, 2015

- 8:00–9:00     *Continental Breakfast*
- 9:00–9:40     **Paul Ayers** (McMaster University)  
*Learning Acid/Base Strength*
- 10:00–10:15   *Break*

*(Friday schedule continued on next page)*

*(Friday schedule continued from previous page)*

- 10:15–10:55 **Pierre Baldi** (University of California, Irvine (UCI))  
*Deep Learning for Many-Particle Systems*
- 11:15–11:30 *Break*
- 11:30–12:10 **George Booth** (King's College London)  
*Stochastic wavefunction compression: Tensor decomposition, Spectra, excited states and more...*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:40 **Robert DiStasio** (Princeton University)  
*Designer Spin Systems via Inverse Statistical Mechanics*
- 3:00–3:15 *Break*
- 3:15–3:55 **Koji Tsuda** (University of Tokyo)  
*Bayesian optimization in materials informatics*

