

## Workshop I: Machine Learning Meets Many-Particle Problems

### Monday September 26, 2016

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–9:50 **Rampi Ramprasad** (University of Connecticut)  
*Machine Learning in Materials Science: Recent Progress and Critical Next Steps*
- 10:00–10:15 *Break*
- 10:15–11:05 **Sameer Varma** (University of South Florida)  
*Discerning protein activity regulation mechanism using “inverse” machine learning*
- 11:15–11:30 *Break*
- 11:30–12:20 **Yousung Jung** (Korea Advanced Institute of Science and Technology (KAIST))  
*Machine learning approaches to the configuration energies and chemisorption models in solids*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Klaus-Robert Müller** (Technische Universität Berlin)  
*Machine Learning meets Quantum Chemistry*
- 3:30–4:00 *Break*
- 4:00–4:50 **Chris Wolverton** (Northwestern University)  
*Using Machine-Learning to Create Predictive Material Property Models*
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

### Tuesday September 27, 2016

- 8:15–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:50 **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne (EPFL))  
*Using machine learning to map the structure and predict the properties of materials and molecules*
- 10:00–10:15 *Break*
- 10:15–11:05 **Anatole von Lilienfeld** (Universität Basel)  
*Quantum Mechanics, Chemical Space, and Machine Learning*
- 11:15–11:30 *Break*

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- 11:30–12:20 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Learning descriptors from materials-science (big) data*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Marco Cuturi** (Kyoto University)  
*Comparing Metric Spaces (and Molecules) with the Gromov-Wasserstein Metric*
- 3:30–4:00 *Break*
- 4:00–4:50 **Volker Roth** (Universität Basel)  
*Archetype analysis: a framework for selecting representative objects*

### Wednesday September 28, 2016

- 8:15–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:50 **José Miguel Hernández-Lobato** (University of Cambridge)  
*Bayesian Optimization for Accelerated Exploration of Chemical Space*
- 10:00–10:15 *Break*
- 10:15–11:05 **Reinhard Maurer** (Yale University)  
*Collective curvilinear coordinates in materials structure search and beyond*
- 11:15–11:30 *Break*
- 11:30–12:20 **Alejandro Rodriguez** (Princeton University)  
*Fluctuation electromagnetic interactions and energy exchange in structured media*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Stefan Tautz** (Forschungszentrum Jülich)  
*Perspectives of Molecular Manipulation and Fabrication*
- 3:30–4:00 *Break*
- 4:00–4:50 **Le Song** (Georgia Institute of Technology)  
*Discriminative Embedding of Molecular Structures for Property Prediction*

### Thursday September 29, 2016

- 8:15–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:50 **Christian Wagner** (Forschungszentrum Jülich)  
*Controlled mechanical manipulation of molecules*
- 10:00–10:15 *Break*

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- 10:15–11:05 **Robert DiStasio** (Cornell University)  
*The Dipole Polarizability of a Condensed-Phase Water Molecule*
- 11:15–11:30 *Break*
- 11:30–12:20 **Isao Tanaka** (Kyoto University)  
*Real and virtual screening for materials discovery through first principles calculations*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Matthias Rupp** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*New dataset, validation experiments, and representation for interpolation across chemical compound space*
- 3:30–4:00 *Break*
- 4:00–4:50 **Panel Discussion**  
*TBA*

### Friday September 30, 2016

- 8:15–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00–9:50 **Koji Tsuda** (University of Tokyo)  
*Machine Learning for Materials Discovery: Low-LTC Compounds, Grain Boundaries, Superlattices and RNAs*
- 10:00–10:15 *Break*
- 10:15–11:05 **Claudia Draxl** (Humboldt-Universität)  
*Big data in materials science: New tools for getting insight into materials properties and functions*
- 11:15 *Conclusion*

