

## Understanding Many-Particle Systems with Machine Learning Tutorials

### Tuesday September 13, 2016

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00–10:15 **Klaus-Robert Müller** (Technische Universität Berlin)  
*Supervised Machine Learning*
- 10:25–10:45 *Break*
- 10:45–12:00 **Alexandre Tkatchenko** (University of Luxembourg)  
*Electronic Structure theory 1*
- 12:00–12:30 *Core Orientation with IPAM Staff*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:45 **Marina Meila** (University of Washington)  
*Unsupervised ML 1*
- 2:55–3:15 *Break*
- 3:15–4:00 **Matthew Hirn** (Michigan State University)  
*Wavelets 1*
- 4:10–4:30 *Break*
- 4:30–5:15 **Kieron Burke** (University of California, Irvine (UCI))  
*DFT 1*

### Wednesday September 14, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:45 **Alexandre Tkatchenko** (University of Luxembourg)  
*Electronic Structure theory 2*
- 9:55–10:15 *Break*
- 10:15–11:00 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)  
*Mathematical representations of quantum states 1*
- 11:10–11:30 *Break*

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- 11:30–12:15 **Glenn Martyna** (IBM Watson Research Center)  
*Stat Mech 1*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:45 **Marina Meila** (University of Washington)  
*Unsupervised ML 2*
- 2:55–3:15 *Break*
- 3:15–4:00 **Matthew Hirn** (Michigan State University)  
*Wavelets 2*
- 4:10–4:30 *Break*
- 4:30–5:15 **Kieron Burke** (University of California, Irvine (UCI))  
*DFT 2*

### Thursday September 15, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:45 **Susan Sinnott** (Pennsylvania State University)  
*Developing and Fitting Reactive Empirical Potentials to Enable Atomic-Scale Simulations*
- 9:55–10:15 *Break*
- 10:15–11:00 **Glenn Martyna** (IBM Watson Research Center)  
*Stat Mech 2*
- 11:10–11:30 *Break*
- 11:30–12:15 **Eric Cancès** (École Nationale des Ponts-et-Chaussées)  
*Mathematical representations of quantum states 2*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–3:15 **Alexander Shapeev** (Skolkovo Institute of Science and Technology)  
*Coarse graining*
- 3:25–3:45 *Break*
- 3:45–5:00 **Gabor Csányi** (University of Cambridge)  
*Gaussian Processes*

## Friday September 16, 2016

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:45 **Susan Sinnott** (Pennsylvania State University)  
*Material Surfaces, Grain Boundaries and Interfaces: Structure-Property Relationship Predictions*
- 9:55–10:15 *Break*
- 10:15–11:00 **Risi Kondor** (University of Chicago)  
*Representation theory, Fourier analysis, and invariants 1*
- 11:00–11:15 *Break*
- 11:15–12:00 **Risi Kondor** (University of Chicago)  
*Representation theory, Fourier analysis, and invariants 2*
- 12:30–2:00 *Lunch (on your own)*
- 2:00–3:15 **Matthias Rupp** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)  
*Practical Tutorial on Machine Learning for Electronic Structure Calculations*

