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*