Workshop I: Optimization and Optimal Control for Complex Energy and Property Landscapes

Monday October 2, 2017

8:00–8:50 *Check-in/Breakfast (hosted by IPAM)*

8:50–9:00 *Welcome and Opening Remarks*

9:00–9:40 **Richard Hennig** (University of Florida)
Optimization and Search of Energy Landscapes by Evolutionary Algorithms and Data Mining

10:00–10:15 *Break*

10:15–10:55 **Luis Nunes Vicente** (University of Coimbra)
A multistart multisplit direct search methodology for global optimization

11:15–11:30 *Break*

11:30–12:10 **Ying Wai Li** (Oak Ridge National Laboratory)
Scalable and efficient multicanonical algorithms for first-principles based Monte Carlo simulations

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Alexey Kolmogorov** (Binghamton University (SUNY))
Systematic development of neural network-based interatomic models for structure prediction

3:30–4:00 *Break*

4:00–4:40 **Lightning Poster Presentations**

5:00–6:30 **Poster Session & Reception**

Tuesday October 3, 2017

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:40 **David Wales** (University of Cambridge)
Energy Landscapes: Structure, Dynamics, and Thermodynamics

10:00–10:15 *Break*

10:15–10:55 **Patrick Avery** (SUNY Buffalo)
Improving Atomistic Crystal Structure Prediction Searches through Symmetric Initialization

11:15–11:30 *Break*

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11:30–12:10 **Logan Ward** (University of Chicago)
Machine learning and global optimization for materials discovery

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Maosheng Miao** (California State University, Northridge (CSU Northridge))
Automatic search versus chemical rules in materials structure study

3:30–4:00 *Break*

4:00–4:40 **Rong Ge** (Duke University)
How to Escape Saddle Points Efficiently?

Wednesday October 4, 2017

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:40 **Ichiro Takeuchi** (University of Maryland)
High-throughput experimentation and machine learning for materials discovery

10:00–10:15 *Break*

10:15–10:55 **Atsuto Seko** (Kyoto University)
Applications of machine learning to materials data

11:15–11:30 *Break*

11:30–12:10 **Luca Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
A meta-machine-learning method for identifying effective descriptors of materials properties

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Bjork Hammer** (Aarhus University)
Local energy decomposition via machine learning

3:30–4:00 *Break*

4:00–4:40 **Yannis Kevrekidis** (Princeton University)
An Equal Space for Complex Data with Unknown Internal Order: Observability, Gauge Invariance and Manifold Learning

Thursday October 5, 2017

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:40 **Christof Schuette** (Freie Universität Berlin)
An Optimal Control Approach to Efficient Estimation of Rare Event Statistics

10:00–10:15 *Break*

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10:15–10:55 **Noa Marom** (Carnegie-Mellon University)
Structure Prediction of Molecular Crystals with GAtor and Genarris

11:15–11:30 *Break*

11:30–12:10 **Anastassia Alexandrova** (University of California, Los Angeles (UCLA))
Ensemble representation of surface-mounted cluster catalysts

12:30–2:30 *Lunch (on your own)*

2:30–3:10 **Karsten Reuter** (Technical University Munich (TUM))
Exploring discrete and continuous landscapes

3:30–4:00 *Break*

4:00–5:00 *Discussion*

Friday October 6, 2017

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00–9:40 **Geoffrey Hutchison** (University of Pittsburgh)
Exploring the Small Molecule Conformer Problem

10:00–10:20 *Break*

10:20–11:00 **Patrick Rinke** (Aalto University)
Human vs Machine: deciphering the structure of organic-inorganic interfaces

11:20–11:35 *Break*

11:35–12:15 **Oliver Hofmann** (Technische Universität Graz)
Surface Adsorbate Polymorph Prediction With Little Effort

12:35–2:30 *Lunch (on your own)*

2:30–3:10 **Nick Sahinidis** (Carnegie-Mellon University)
ALAMO: Machine learning from data and first principles

3:30–4:00 *Break*

4:00–4:40 **Stephen Wright** (University of Wisconsin-Madison)
Algorithmic Tools for Smooth Nonconvex Optimization

5:00 *Conclusion*