

## 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*

