

Learning and Emergence in Molecular Systems

Monday January 23, 2023

- 8:00–8:55 *Check-in/Breakfast (hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00 *Session Chair: Xavier Bresson (National University of Singapore)*
- 9:00–9:50 **Frank Noe** (Freie Universität Berlin)
Advancing molecular simulation with deep learning
- 10:00–10:15 *Break*
- 10:15–11:05 **Patrick Riley** (Relay Therapeutics)
Symbolic Regression for Discovery of a DFT Functional
- 11:15–11:30 *Break*
- 11:30–12:20 **Mohammed AlQuraishi** (Harvard Medical School)
OpenFold: Lesson learned and insights gained from rebuilding and retraining AlphaFold2
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Alex Tkatchenko (University of Luxembourg)*
- 2:30–3:20 **Cecilia Clementi** (Freie Universität Berlin)
Coarse-graining classical and quantum systems
- 3:30–4:00 *Break*
- 4:00–4:50 **Payel Das** (IBM Research)
Design and Evaluation of Foundation Models and Generative AI in Molecular Space
- 5:00–5:15 *Lightning Poster Presentations*
- 5:15–6:45 *Poster Session & Reception (Hosted by IPAM)*

Tuesday January 24, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *Session Chair: Steve Brunton (University of Washington)*
- 9:00–9:50 **Steve Brunton** (University of Washington)
Machine Learning for Scientific Discovery, with Examples in Fluid Mechanics
- 10:00–10:15 *Break*

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- 10:15–11:05 **Rafael Gomez-Bombarelli** (Massachusetts Institute of Technology)
End-to-end learning and auto-differentiation: forces, uncertainties, observables, trajectories and scales.
- 11:15–11:30 *Break*
- 11:30–12:20 **Kristin Persson** (University of California, Berkeley (UC Berkeley))
Data-Driven Design for Energy Materials
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Cecilia Clementi (Freie Universität Berlin)*
- 2:30–3:20 **Tommi Jaakkola** (Massachusetts Institute of Technology)
Virtual Talk: Diffusion based distributional modeling of conformers, blind docking and proteins
- 3:30–4:00 *Break*
- 4:00–4:50 **Mark Tuckerman** (New York University)
From A to B via a synthesis of rare-event sampling and machine learning

Wednesday January 25, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *Session Chair: Patrick Riley (Relay Therapeutics)*
- 9:00–9:50 **Max Welling** (Microsoft Research)
Learning and Emergence in Molecules and Brains
- 10:00–10:15 *Break*
- 10:15–11:05 **Xavier Bresson** (National University of Singapore)
Graph MLP-Mixer for Molecular Analysis
- 11:15–11:30 *Break*
- 11:30–12:20 **Alexandre Tkatchenko** (University of Luxembourg)
Fully Quantum (Bio)Molecular Simulations: Dream or Reality?
- 12:30–12:45 *Group Photo Session*
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: : Jutta Rogal (New York University)*
- 2:30–3:20 **Stefan Chmiela** (Technische Universität Berlin)
Accurate global machine learning force fields for molecules with hundreds of atoms
- 3:30–4:00 *Break*
- 4:00–4:50 **Kyunghyun Cho** (New York University)
Lab-in-the-loop de novo antibody design - what are we missing from machine learning?

Thursday January 26, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *Session Chair: Max Welling (Microsoft Research)*
- 9:00–9:50 **Tess Smidt** (Massachusetts Institute of Technology)
Symmetry's made to be broken: Learning how to break symmetry with symmetry-preserving neural networks
- 10:00–10:15 *Break*
- 10:15–11:05 **Bruno Correia** (École Polytechnique Fédérale de Lausanne (EPFL))
Virtual Talk: Exploring new molecular representations for the design of biological function
- 11:15–11:30 *Break*
- 11:30–12:20 **Jutta Rogal** (New York University)
Pathways in classification space - Machine learning collective variables for enhanced sampling of structural transformations
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Stefan Chmiela (Technische Universität Berlin)*
- 2:30–3:20 **Kyle Cranmer** (University of Wisconsin-Madison)
Connections and cross pollination from quarks to the cosmos
- 3:30–4:00 *Break*
- 4:00–4:50 **Rose Yu** (University of California, San Diego (UCSD))
Incorporating Symmetry for Learning Spatiotemporal Dynamics

Friday January 27, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *Session Chair: Frank Noe (Freie Universität Berlin)*
- 9:00–9:50 **Maxim Ziatdinov** (Oak Ridge National Laboratory)
Exploring the Intersection of Machine Learning and Electron Microscopy: Advances in Automated Experiments and Physics Discovery
- 10:00–10:15 *Break*
- 10:15–11:05 **Ron Dror** (Stanford University)
Virtual Talk: Leveraging small datasets for molecular machine learning
- 11:15–11:30 *Break*
- 11:30–12:20 **Anatole von Lilienfeld** (University of Toronto)
Virtual Talk: Go EAST, young scientist - First principles view on chemical compound space

