Advancing Quantum Mechanics with Mathematics and Statistics Reunion Conference 2

Sunday December 8, 2024

1:30 *Bus Departs UCLA/Faculty Center*

4:30 *Check in at Lake Arrowhead*

6:30–8:00 *Dinner*

8:00–9:00 *Joint Session: Jacob Foster (MOILA), Jan Janssen (NMERC1), Eric Cances (QMMRC2)*

9:00–10:00 *Social Hour (Iris)*

Monday December 9, 2024

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

9:00–9:40 **Kieron Burke** (University of California, Irvine (UCI))
DFT and ML

10:00–10:20 **Abigail Poteshman** (University of Chicago)
High-throughput nuclear spin-bath characterization of defects in semiconductors using trans-dimensional Bayesian model selection

10:30–10:50 **Trine Quady** (University of California, Berkeley (UC Berkeley))
Method-independent approach to cusp Gaussian-type orbitals applied to variational Monte Carlo

11:10–11:50 **Philip Kurian** (Howard University)
Non-Hermitian Hamiltonians for biological qubit-light interfaces

12:00–1:00 *Lunch (hosted by IPAM)*

2:00–2:40 **Jason Gibson** (Los Alamos National Laboratory)
Developing a Complete AI-Accelerated Workflow for Superconductor Discovery

3:00–3:20 **Mihail Bogojeski** (Technische Universität Berlin)
Equivariant Neural Networks for Orbital-Free Density Functional Theory

3:30–4:00 **Marcel Langer** (École Polytechnique Fédérale de Lausanne (EPFL))
Considering the role of physical constraints in machine learning potentials

4:00–4:20 **Guido Falk von Rudorff** (University of Vienna)
Uniform Random Sampling of Chemical Space

6:30–8:00 *Dinner*

8:00–8:50 *Joint Session: Klaus-Robert Mueller (QMMRC2)*

9:00–10:00 *Social Hour (Iris)*

Tuesday December 10, 2024

8:00–9:00	*Check-in/Breakfast (hosted by IPAM)*
9:00–9:40	**Sambit Das** (University of Michigan) *Pushing the length-scale and accuracy frontier of DFT calculations: application to quasicrystal energetics.*
10:00–10:40	**Volker Blum** (Duke University) *Scaling advances and new functionality in FHI-aims*
11:00–11:20	**Vincent Martinetto** (University of California, Merced (UC Merced)) *A demonstration of the Finite-Temperature Upside-Down Adiabatic Connection with the Asymmetric Hubbard Dimer*
11:30–11:50	**Christopher Sutton** (University of South Carolina) *TBD*
12:00–1:00	*Lunch (hosted by IPAM)*
1:00–5:00	*Afternoon Free*
6:30–8:00	*Dinner*
8:00–8:50	*Joint Session: Ida Momennejad (MOILA)*
9:00–10:00	*Social Hour (Iris)*

Wednesday December 11, 2024

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

9:00–9:40 **Eric Cances** (École Nationale des Ponts-et-Chaussées)
TBD

10:00–10:20 **Kevin Stubbs** (Duke University)
TBD

10:30–10:50 **Brian Ernst** (Cornell University)
NENCI-2021: A large benchmark database of non-equilibrium non-covalent interactions emphasizing close intermolecular contacts

11:00–11:20 **Fabian Faulstich** (Rensselaer Polytechnic Institute)
Algebraic varieties in coupled cluster theory for quantum chemistry

11:30–11:50 **Gil Goldshlager** (University of California, Berkeley (UC Berkeley))
Some thoughts on training neural networks to represent scientific functions

12:00–1:00 *Lunch (hosted by IPAM)*

2:00–2:20 **Ping Yang** (Los Alamos National Laboratory)
Enabling Separation Sciences via Complex Computational Workflow

2:30–2:50 **Stefan Chmiela** (Technische Universität Berlin)
Addressing Many-Body Effects in Machine-Learning Force Fields

3:00–3:40 **Almaz Khabibrakhmanov** (University of Luxembourg)
Noncovalent Interactions in Density Functional Theory: All the Charge Density We Do Not See

3:40–4:20 *TBA*

6:30–8:00 *Dinner*

8:00–8:50 *Joint Session: Thomas Swinburne (NMERC1)*

9:00–10:00 *Social Hour (Iris)*

Thursday December 12, 2024

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

9:00–9:40 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung GmbH)
pyiron as a workflow language: Concepts and application to ab initio thermodynamics

10:00–10:20 **Mira Todorova** (Max-Planck-Institut für Eisenforschung GmbH)
Applying automated computational workflows to obtain reaction barriers in electrochemical systems

10:30–10:50 **Jagannath Mantha** (University of Texas at Austin)
Formation of Two-Level Systems (TLS) at Interfaces in Nb-based Transmon Qubits

11:10–11:50 **Robert DiStasio** (Cornell University)
TBD

12:00–1:00 *Lunch (hosted by IPAM)*

4:30–4:50 **Zachary Sparrow** (Cornell University)
Construction and Analysis of the NECE-2024 Benchmark Non-Equilibrium Conformational Energy Database

5:00–5:20 **Matteo Gori** (University of Luxembourg)
TBD

5:30–5:50 **Kangbo Li** (Cornell University)
The Semantics of Second Quantization

6:00–6:20 **Lucas Tecot** (University of California, Los Angeles (UCLA))
Provably Noise-Resilient Training of Parameterized Quantum Circuits

6:30–8:00 *Dinner*

9:00–10:00 *Social Hour (Iris)*

Friday December 13, 2024

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

9:00–12:00 *Discussion*

12:00–1:00 *Lunch (hosted by IPAM)*

1:30 *Bus Departs Lake Arrowhead (LAX/Marriott/UCLA)*

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