Workshop I: Multiscale Approaches in Quantum Mechanics

Monday March 28, 2022

8:00–8:55 *Check-In/Light 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)*

9:00–9:50 **Alexandre Tkatchenko** (University of Luxembourg)
Multiscale Approaches to Quantum Mechanics: From Vacuum, to Atoms, to Engineering-Scale Structures

10:00–10:15 *Break*

10:15–11:05 **Giulia Galli** (University of Chicago)
Embedding theories for quantum simulations on hybrid classical-quantum architectures

11:15–11:30 *Break*

11:30–12:20 **Angel Rubio** (Max Planck Institute for the Structure and Dynamics of Matter)
Virtual Talk: Polaritonic Quantum Materials: a first principles QEDFT perspective

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Dominika Zgid** (University of Michigan)
Post-DFT Green's function embedding

3:30–3:45 *Break*

3:45–4:35 **Michael Lindsey** (Courant Institute of Mathematical Sciences)
Virtual talk: Quantum embedding with lower bounds

4:45–5:10 *Lightning Poster Session*

5:10–6:45 *Poster Session & Reception (Hosted by IPAM)*

Tuesday March 29, 2022

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

10:00–10:15 *Break*

10:15–11:05 **Andrew Millis** (Columbia University)
Virtual Talk: Twisted Transition Metal Dicalcogenides: Experimental Tests of Quantum Embedding and Theories

11:15–11:30 *Break*

(Tuesday schedule continued on next page)

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11:30–12:20 **Christoph Ortner** (University of British Columbia)
Modelling Atomic Properties with the Atomic Cluster Expansion

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Gero Friesecke** (Technische Universität München)
Fast algorithm for the strong-interaction limit of density functional theory

3:30–4:00 *Break*

4:00–4:50 **Reinhold Schneider** (Technische Universität Berlin)
Tensor Networks (QC-DMRG) in a Complete Active Space Coupled Cluster Method

Wednesday March 30, 2022

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:50 **Prineha Narang** (Harvard University)
TBA

10:00–10:15 *Break*

10:15–11:05 **Laura Gagliardi** (University of Chicago)
Virtual Talk: Localized-Wave-Function Methods in Quantum Chemistry and Their Extension to Quantum Computers

11:15–11:30 *Break*

11:30–12:20 **Michael Weinstein** (Columbia University)
Virtual Talk: Discrete honeycombs, rational edges and edge states

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Mitchell Luskin** (University of Minnesota, Twin Cities)
Electronic Observables for Relaxed 2D van der Waals Heterostructures at the Moiré Scale

3:30–4:00 *Break*

4:00–4:50 **Hakan Tureci** (Princeton University)
Virtual talk: Quantum electrodynamic modeling of superconducting quantum systems

Thursday March 31, 2022

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:50 **Alejandro Rodriguez** (Princeton University)
Virtual Talk: Physical bounds on wave phenomena as quadratically constrained quadratic programs

10:00–10:15 *Break*

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10:15–11:05 **Marco Govoni** (Argonne National Laboratory)
Code interoperability extends the scope of first principles spectroscopy

11:15–11:30 *Break*

11:30–12:20 **Jianfeng Lu** (Duke University)
Virtual Talk: Taming the dynamical sign problem in diagrammatic algorithms for open quantum systems

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Fabian Faulstich** (University of California, Berkeley (UC Berkeley))
On the pure state v-representability of density matrix embedding theory—an augmented lagrangian approach

3:30–4:00 *Break*

4:00–4:50 **Stefan Chmiela** (Technische Universität Berlin)
Non-locality in machine learning force fields

Friday April 1, 2022

8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*

9:00–9:50 **Martin Stöhr** (University of Luxembourg)
Why More is Different: The (Non-)Scalability of Approximations in Modeling Non-covalent Interactions

10:00–10:15 *Break*

10:15–11:05 **George Booth** (King's College London)
Virtual Talk: A rigorous framework for embedding realistic interacting quantum systems

11:15–11:30 *Break*

11:30–12:20 **Matteo Gori** (University of Luxembourg)
Second-Quantization of Many-Body Dispersion Formalism: Towards Modeling of Million Atom Systems in Arbitrary Environments

12:30–2:30 *Lunch (on your own)*

2:30–2:50 **Mihail Bogojeski** (Technische Universität Berlin)
Message passing neural networks for atomistic systems: Molecules

3:00–3:20 **Marcel Langer** (Technische Universität Berlin)
Message passing neural networks for atomistic systems: Materials

3:30–4:00 *Break*

4:00–4:50 **Timothy Gould** (Griffith University)
Virtual Talk: Multiscale approaches to dispersion modelling