Advancing Quantum Mechanics with Mathematics and Statistics

Tuesday March 15, 2022

2:30–3:00 **Brian Ernst** (Cornell University)
Some applications of density functional theory to organic chemistry

3:00–3:30 *Tea Time*

3:30–4:00 **Kevin Stubbs** (University of California, Los Angeles (UCLA))
A Mathematical Perspective on Wannier Functions

Thursday March 17, 2022

2:30–3:00 **Szabolcs Góger** (University of Luxembourg)
Non-Local Polarizability Densities for van der Waals Interactions

3:00–3:30 *Tea Time*

3:30–4:00 **Zeno Schätzle** (Freie Universität Berlin)
PauliNet: A deep-neural-network trial wave function for variational Quantum Monte Carlo

Tuesday March 22, 2022

2:30–3:00 **Marcel Langer** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Thermal Transport with Message-Passing Neural Networks and the Green-Kubo Method

3:00–3:30 *Tea Time*

3:30–4:00 **Max Pfeffer** (Technische Universität Chemnitz)
Particle number conservation and block structures in Matrix Product States

Wednesday March 23, 2022

2:00–3:00 **Oleg Prezhdo** (University of Southern California (USC))
Guest Speaker: Nonadiabatic Molecular Dynamics of Nanoscale Systems

3:00–3:30 *Tea Time*

4:00–5:00 **Rafael Lainez Reyes** (University of California, Santa Barbara (UCSB))
TUTORIAL: Hartree-Fock and Self Consistent Iteration

Thursday March 24, 2022

2:30–3:00 **Mihail Bogojeski** (Technische Universität Berlin)
Machine learning for electronic structure

3:00–3:30 *Tea Time*

3:30–4:00 **Gil Goldshlager** (University of California, Berkeley (UC Berkeley))
Neural network representations for antisymmetric functions

Tuesday April 5, 2022

2:30–3:00 **Abigail Poteshman** (University of Chicago)
Recovering hyperfine interactions in random nuclear spin baths

3:00–3:30 *Tea Time*

3:30–2:00 **Kangbo Li** (Cornell University)
PBC and Wannier functions

Thursday April 7, 2022

2:30–3:00 **Muhammad Hassan** (Université de Paris VI (Pierre et Marie Curie))
Approximating Energy Bands in the Brillouin Zone

3:00–3:30 *Tea Time*

3:30–4:00 **Kangbo Li** (Cornell University)
A Taste of Julia

Tuesday April 19, 2022

2:30–3:00 **Eloïse Letournel** (École Nationale des Ponts-et-Chaussées (ENPC))

3:00–3:30 *Tea Time*

Tuesday April 26, 2022

3:30–4:00 **Almaz Khabibrakhmanov** (University of Luxembourg)
Towards the Universal van der Waals Potential

Wednesday April 27, 2022

2:00–3:00 **Troy van Voorhis** (Massachusetts Institute of Technology)
Guest Speaker: Title TBD

Thursday April 28, 2022

2:30–3:00 **Gaspard Kemlin** (École des Ponts ParisTech)
Practical error bounds for properties in plane-wave electronic structure calculations

Tuesday May 10, 2022

10:00–11:00 **Mihail Bogojeski** (Technische Universität Berlin)
[ML Mini-WS] Equivariant Neural Networks

2:00–3:00 **Jack Thomas** (University of Warwick)
[ML Mini-WS] Physics-Informed Models

Wednesday May 11, 2022

10:00–11:00 **Jan Thorben Frank** (Technische Universität Berlin)
[ML Mini-WS] Geometric Attention

2:00–3:00 **Adil Kabylda** (University of Luxembourg)
[ML Mini-WS] Long-Range Interactions

Thursday May 12, 2022

10:00–11:00 **Yangshuai Wang** (University of British Columbia)
[ML Mini-WS] Error Propagation

2:00–3:00 **Alice Allen** (University of Luxembourg)
[ML Mini-WS] Machine learning of material properties: Predictive and interpretable multilinear models

3:00–3:30 *Tea Time*

Tuesday May 17, 2022

2:30–3:00 **Zachary Sparrow** (Cornell University)
Towards Routine Use of Hybrid DFT for Large-Scale Finite-Gap Condensed-Phase Systems

3:00–3:30 *Tea Time*

Wednesday May 18, 2022

8:00 *QM 2D Moiré Scale Mini-Workshop (May 18-20)*

8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:15 *QM Moiré Scale Mini-Workshop Introduction*

9:15–10:30 **Stephen Carr** (Brown University)
QM Moiré Scale Mini-Workshop: An introduction to 2D materials and Moiré physics

10:30–11:00 *Break*

11:00–12:15 **Maciej Zworski** (University of California, Berkeley (UC Berkeley))
QM Moiré Scale Mini-Workshop: Spectral theory of the chiral model of TBG

12:15–2:00 *Lunch (on your own)*

2:00–3:15 **Allan MacDonald** (University of Texas at Austin)
QM Moiré Scale Mini-Workshop: Moire Materials Models

3:15–3:30 *Break*

3:30–4:45 **Lin Lin** (University of California, Berkeley (UC Berkeley))
QM Moiré Scale Mini-Workshop: Interacting models for twisted bilayer graphene

Thursday May 19, 2022

8:00 *QM 2D Moiré Scale Mini-Workshop (May 18-20)*

8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–10:15 **Michael Zaletel** (University of California, Berkeley (UC Berkeley))
QM Moiré Scale Mini-Workshop: The strong-coupling theory of magic-angle graphene

10:15–10:30 *Break*

(Thursday schedule continued on next page)

(Thursday schedule continued from previous page)

10:30–11:45 **Svetlana Jitomirskaya** (University of California, Irvine (UCI))
QM Moiré Scale Mini-Workshop: Opening and closing of the gaps in the extended Harper's model

12:00–2:00 *Lunch (on your own)*

2:00–3:15 **Alexander Watson** (University of Minnesota, Twin Cities)
QM Moiré Scale Mini-Workshop: Justification of the BM model and WKB construction of flat band wavefunctions

3:15–3:30 *Break*

3:30–4:45 **Eric Cances** (École Nationale des Ponts-et-Chaussées)
QM Moiré Scale Mini-Workshop: From Kohn-Sham to Bistritzer-MacDonald and related models

Friday May 20, 2022

8:00 *QM 2D Moiré Scale Mini-Workshop (May 18-20)*

8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*

10:15–10:30 *Break*

10:30–11:45 **Mitchell Luskin** (University of Minnesota, Twin Cities)
QM Moiré Scale Mini-Workshop: A framework for the electronic structure and mechanical relaxation of 2D multilayer heterostructures

12:00–2:00 *Lunch (on your own)*

2:00–3:15 **Ziyan Zhu** (Harvard University)
QM Moiré Scale Mini-Workshop: Low-energy moiré phonons in twisted bilayer van der Waals heterostructures

3:15–3:30 *Break*

3:30–4:45 **Stephen Carr** (Brown University)
QM Moiré Scale Mini-Workshop: Seeing Moiré: Learning twistronics with a convolutional neural net