Telluride Workshop: Multi-Scale Quantum Mechanical Analysis of Condensed Phase Systems: Methods and Applications

July 8-11, 2022
Organizers: Ben Hourahine (University of Strathclyde), Anders Niklasson (LANL), Tim Kowalczyk (Western Washington University), David Yaron (Carnegie Melon University), Nir Goldman (LLNL)

Location: Telluride Intermediate School, 725 West Colorado Ave Telluride CO, 81435

July 8, Monday: General Methodologies (Session Chair: Ben Hourahine)
8:00-9:00 AM Breakfast
9:00-9:20 Introductory remarks (All of us)
9:20-10:00 Weitao Yang (Duke), *"QM/MM, Machine Learning and DFT for Excited States"*
10:00-10:40 Jonathan Moussa (MolSSI), *"My technical roadmap for semiempirical electronic structure"*
10:40-11:00 Coffee Break
11:00-11:40 Stephan Irle (ORNL), *"Harnessing the Power of Supercomputers and AI for Molecular and Materials Design"*
11:40-12:20 Tomáš Kubař (KIT), *"Simulation of reactions in biomolecular complexes: Blending the flavors"*

12:10-2:00 PM Lunch
(Session Chair: David Yaron)
2:00-2:40 Anders Niklasson (LANL), *"Next Generation Quantum-Mechanical Molecular Dynamics Simulations with Tens-of-Thousands of Atoms"*
2:40-3:20 Kevin Garrity (NIST), *"Three-body tight binding for the periodic table"*
3:20-4:00 Christoph Bannwarth (Aachen), *"Recent Developments for Semiempirical Electronic Structure Theory: Application, Modularization, and Acceleration on Commodity Hardware"*

July 9, Tuesday: Methodologies II (Session Chair: Tim Kowalczyk)
8:00-9:00 AM Breakfast
9:00-9:40 Qiang Cui (Boston University), *"Exploration of machine learning methods and the effect of electronic polarization in biomolecular simulations"*
9:40-10:20 Sergei Tretiak, *"Applications of non-adiabatic excited state molecular dynamics to molecular systems"*
10:20-11:00 Van Quan Vuong (KIT), *"Multipole Expansion in Density-Functional Tight-Binding: Current Progress and Future Plans"*
11:00-11:20 Coffee Break
Machine-Learning Developments and Enhancements of Electronic Structure Calculations I (Session chair: Tim Kowalczyk)
11:20-12:00 David Yaron (CMU), *"Quantum chemical Hamiltonians as flexible and interpretable model forms for machine learning"*

12:00-12:40 Shuwen Yue (Cornell), *"Physics-inspired machine learning potentials for thermodynamic and dynamic properties of electrolyte solutions"*
Lunch, Group hike(s)
Town Talk

July 10, Wednesday: Machine-Learning Developments and Enhancements of Electronic Structure Calculations II (Session Chair: David Yaron)
8:00-9:00 AM Breakfast
9:00-9:40 Kieron Burke (UC Irvine), *"Recent developments in density functional approximations"*
9:40-10:20 Bálint Aradi (Bremen), *"DFTB & Machine Learning: Current Approaches and Perspectives"*
10:20-10:40 Coffee Break
(Session Chair: Anders Niklasson)
10:40-11:20 Justin Smith (Nvidia), *"Improving the applicability and efficiency of AI for atomistic simulation"*
11:20-12:00 Adam Mcsloy (Bristol), *"TBMaLT, a Flexible Toolkit for Combining Tight-Binding and Machine Learning"*
12:00-2:00 Lunch

Materials and Applications I (Session Chair: Anders Niklasson)
2:00-2:40 Ben Hourahine (Strathclyde) *"Thoughts about testing future semi-empirical methods"*
2:40-3:20 Nir Goldman (LLNL), *"Sampling Chebyshev Clusters to Create Systematically Improvable DFTB Models"*
3:20-4:00 Bryan Wong (UC Riverside), "*Probing Electron Dynamics of Complex Material Systems in Real Time"*

July 11, Thursday: Materials and Applications II (Session Chair: Nir Goldman)
8:00-9:00 AM Breakfast
9:00-9:40 Tim Kowalczyk (WWU), *"Tight-binding simulation of excitation-driven function in porous organic frameworks and metal nanocubes"*
9:40-10:20 Roman Zubatiuk (CMU), *"AIMNet2 family of machine learning potentials: general-purpose and task-specific models for element-organic molecules and radicals, reactions and molecular crystals"*
10:20-11:00 Tammo van der Heide (Bremen), "*Hybrid Functionals for Periodic Systems in the Density Functional Tight-Binding Method"*
11:00-2:00 Concluding Discussions and Lunch

Additional Events

Sunday, July 7, 5:00pm to 6:30pm
All-Telluride Science Meet and Greet
Location: Alibi – 157 S. Fir Street
This is a good chance to meet up with fellow participants before your meeting. A staff member will be on hand to welcome you and distribute badges.
**Please note that this is a NEW location for our Meet & Greet.*

Wednesday, July 10 5:30pm - 7:30pm
All Telluride Science Picinic
Free BBQ, Beer, Wine, and Non-Alcoholic Beverages. Friends and Family are invited free of charge.
Location: Tent behind the Intermediate School (*which is the location for all workshops - 725 W Colorado Ave*)