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

July 12-16, 2022
Organizers: Nir Goldman (LLNL), Ben Hourahine (University of Strathclyde), Anders Niklasson (LANL), Tim Kowalczyk (Western Washington University), David Yaron (Carnegie Melon University)

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

July 12, Tuesday: General Methodologies (Session Chair: Nir Goldman)
8:00-9:00 AM Breakfast
9:00-9:10 Introductory remarks from Nir
9:10-9:50 Stefan Grimme “A new tight-binding electronic structure method in a polarized valence double-zeta basis set for the spd-block elements Z=1-86”
9:50-10:30 Anders Niklasson "Quantum-based molecular dynamics using deep neural networks and AI hardware"
10:30-10:50 Coffee Break

10:50-11:30 Ben Hourahine, “Minimal and sub-minimal basis semi-empirical DFT”
11:30-12:10 Xin Xing, “Finite-size error and its correction in energy calculations for periodic systems”
12:10-2:00 PM Lunch

2:00-2:40 Chris Skylaris, “Methods for electrochemistry simulations of metallic systems within a local orbital linear-scaling DFT framework”
2:40-3:20 Qiang Cui, “DFTB based QM/MM methods: developments and applications”
Break early for hiking, etc.

July 13, Wednesday: Machine-Learning Developments and Enhancements of Electronic Structure Calculations I (Session Chair: Ben Hourahine)
8:00-9:00 AM Breakfast
9:00-9:40 Marivi Fernandez-Serra, “Machine learning approaches to improve the exchange and correlation functional in DFT”
9:40-10:20 Huy Pham, “Development of Semiempirical Quantum Models with High Accuracy and Minimal Training Set Using Chebyshev Polynomial-Based Force Fields”
10:20-10:40 Coffee Break

10:40-11:20 David Yaron, “Learned Hamiltonians as Interpretable Machine Learning Models of Chemical Systems”
11:20-12:00 Johannes Margraf, “Δ-Learning with DFTB: What makes a good baseline?”

Lightning Talks:
12:00-12:05 Gang Seob Jung, “Parameterizations of DFTB and neural network potentials for rare event simulations”
12:05-12:10 Pilsun Yoo, “Computational vibrational spectroscopic study of coal materials using DFTB”
Lunch, Group hike(s)

July 14, Thursday: Machine-Learning Developments and Enhancements of Electronic Structure Calculations II (Session Chair: David Yaron)
8:00-9:00 AM Breakfast
9:00-9:40 Lorenzo Gigli, “A unified Machine Learning framework for thermodynamic and dielectric properties of ferroelectrics”
9:40-10:20 Sergei Tretiak, “Machine Learning for Molecular Properties: Going Beyond Interatomic Potentials”
10:20-10:40 Coffee Break

Materials and Applications I (Session Chair: Tim Kowalczyk)
10:40-11:20 Giulia Galli, “Quantum embedding for heterogeneous materials”
11:20-12:00 Stephan Irle, “Development and Application of Density-Functional Tight-Binding Methods for Chemical Energy Sciences”
12:00-2:00 Lunch

2:00-2:40 Jianli Cheng, “Materials Design Principles of Amorphous Cathode Coatings for Lithium-Ion Batteries”
2:40-3:20 Chao Zhang, “Finite-field DFTMD modelling of the protonic double layer and beyond”
3:20-4:00 Thomas Niehaus, “Machine learned repulsive potentials for Silicon in the DFTB framework”
Break early for hiking, etc.

July 15, Friday: Materials and Applications II (Session Chair: Anders Niklasson)
8:00-9:00 AM Breakfast
9:00-9:40 Tim Kowalczyk, “Time-independent DFTB perspectives on chromophore emission in complex environments”
9:40-10:20 Yu Zhang, “Non-adiabatic molecular dynamics of light-matter interaction mediated photochemistry”
10:20-11:00 Nir Goldman, “Development of Multi-scale Computational Methodologies for Reactive Materials”
11:00 Coffee and Concluding Discussion