Telluride workshop: Multi-scale quantum mechanical analysis of condensed phase systems: methods and applications

Jul 23-27, 2018
Organizers: Guohui Li (Dalian Institute of Chemical Physics, PRChina), Darrin York (Rutgers), Marcus Elstner (KIT, Germany) and Qiang Cui (Boston Univ.)

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

Jul. 22 Sun. Arrival

Sunday evening get together: TBA

Jul. 23 Mon. Session I: General Methodologies [7]
8:00 – 8:30 AM Breakfast

8:30 – 8:40 AM Brief Intro from Mark and QC

8:40 – 9:20 AM Greg Beran, UC-Riverside, "Solving Molecular Crystal Structures and Phase Diagrams with Ab Initio Fragment Techniques"

9:20 – 10:00 AM Lyudmila Slipchenko, Purdue, "Effective Fragment Potential method: New avenues, new tools"

10:00 – 10:20 AM Coffee Break

10:20 – 11:00 AM Thomas Wesolowski, University of Geneva, "Induction, dispersion, exchange-repulsion, where they are in Frozen-Density Embedding Theory based simulations"

11:00 – 11:40 AM Andrew Simmonett, NIH, "Algorithms for treating long-range interactions"

11:40 AM – 12:20 PM Darrin York, Rutgers, "Linear Scaling QM"

12:20 PM – 2:00 PM Lunch

2:00 – 2:40 PM Thomas Frauenheim, Bremen, TBA

2:40 – 3:20 PM Anders Niklasson, LANL, "Shadow Hamiltonian dynamics for non-linear self-consistent field models"

3:20 – 4:00 PM Robert Rüger, SCM, "The Amsterdam Modeling Suite as a software platform for scientific innovation"

Jul. 24 Tues. Session II: Excitation and Transport [5]
8:00 – 8:30 AM Breakfast

8:30 – 9:10 AM Thomas Niehaus, Lyon, "Towards thermoelectricity with DFTB - Accuracy of phonon band structures"

9:10– 9:50 AM Zhigang Shuai, Tsinghua, "Combined TD-DMRG/TD-HF approach to electronic and optical processes in molecular aggregates"

9:50-10:10 AM Coffee Break

10:10 – 10:50 AM Alexander Humeniuk, Wuerzburg University, "Non-adiabatic molecular dynamics with long-range corrected tight-binding DFT"

10:50 – 11:30 AM Sergei Tretiak, LANL, "The NEXMD computational framework for non-adiabatic excited state dynamics in large molecules"

11:30 – 12:10 PM Chi Yun Yam, Beijing Computational Science Research Center, "Quantum Mechanical Simulations of Light Emission in Nanoscale Devices"

Afternoon: Lunch, Hiking

6:30 PM Town talk (Telluride Conference Center in Mountain Village) – "Geo-Engineering a Climate Change Solution", Frank N Keutsch, Professor of Chemistry and Chemical Biology, Harvard University

Jul. 25 Weds. Session III: DFTB developments [8]
8:00 – 8:30 AM Breakfast

8:30 – 9:10 AM Honza Rezac, Prague, "Modelling biomolecules with approximate QM methods: non-covalent interactions and beyond"

9:10 – 9:50 AM Marcus Elstner, KIT, "Machine learning potentials and weak interactions in DFTB"

9:50 – 10:10 AM Coffee Break

10:10 – 10:50 AM Ben Nebgan, LANL, "Machines learning quantum chemistry: potentials, properties, and p-orbitals"

10:50 – 11:30 AM Goldman Nir, LLNL, "Use of Many-body Force-fields to Accelerate Quantum Simulations of Reactive Materials"

11:30 – 12:10 PM Maja Gruden, Belgrade, "Spinning around in TM chemistry"

12:10 – 2:00 PM Lunch

2:00 – 2:40 PM Ben Hourahine, University of Strathclyde, “Alternative solvers in DFTB+”

2:40 – 3:20 PM Stephane Irle, ORNL, “Replica-exchange umbrella sampling in FMO-DFTB molecular dynamics: Methods and applications”

3:20 – 4:00 PM Christian Negre, LANL, “Extending Quantum Molecular Dynamics to the Exascale: LATTE, PROGRESS and BML Libraries”

6:00 PM Picnic (Tent behind Middle School)

Jul. 26 Thurs. Session IV: Biological Models & Applications [8]
8:00 – 8:30 AM Breakfast

8:30 – 9:10 AM Heather Kulik, MIT, “Systematic approaches to identifying quantum mechanical effects in enzymatic rate enhancement”

9:10 – 9:50 AM Lu Wang, Rutgers, “Structural Characteristics and Quantum Effects in Biological Short Hydrogen Bonds”

9:50 – 10:10 AM Coffee Break

10:10 – 10:50 AM John Herbert, Ohio State, “Quantum chemistry in arbitrary dielectric environments”

10:50 -11: 30 AM Lee Woodcock, Univ. South Florida, “Obtaining Accurate QM/MM Free Energies Using Novel Sampling and Reweighting Approaches”

11:30 -12:10 PM Guohui Li, DICP, “Polarizable model for lipids and integrated accelerate MD”

12:10 – 2:00 PM Lunch

2:00 – 2:40 PM Kwangho Nam, UT-Arlington, “Multiscale Simulation Studies of Catalytic and Allosteric Mechanisms of Protein Kinases”

2:40 – 3:20 PM Ono Junichi, Waseda, “Divide-and-Conquer density-functional tight-binding molecular dynamics simulations for the primary proton transfer in bacteriorhodopsin”

3:20 – 4:00 PM Qiang Cui, BU, “Update of metal ions with DFTB and application to metalloenzymes”

4:00 PM Coffee and Concluding Discussion.

Jul. 27 Fri.

8:00 – 8:30 AM – Breakfast at Telluride Middle school.

9:00 AM – Departure/hiking