

2023 "Computational Materials Chemistry" Telluride Workshop
Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
Monday morning, 17 July 2023 to Friday noon, 21 July 2021; Breakfast starts 7:30am at School

Monday, 17 July 2023

8:00am-8:10am opening remarks

Session I: Reaction networks, modes, and machine learning; Chairs: De-en Jiang/Mira Todorova

8:10am-9:00am Karsten Reuter: Exploring Catalytic Reaction Networks with Machine Learning

9:00am-9:50am Paul Zimmerman: Varieties of Reaction Modes

9:50am-10:20am Coffee Break

10:20am-11:10am Zachary Ulissi: Large generalizable ML potentials for surface reactions

11:10am-12:00pm Bjørk Hammer: Active and reinforcement learning for global optimization

Tuesday, 18 July 2023

Session II: Reactions in water; Chairs: Graeme Henkelman/Karsten Reuter

8:10am-9:00am Yujie Sun: Dual hydrogen evolution and hydrogenation using Pd membrane electrodes

9:00am-9:50am Líney Árnadóttir: Role of water in decomposition of small oxygenates on metal surfaces

9:50am-10:20am Coffee Break

10:20am-11:10am Bin Wang: Water-promoted hydrogenation and C-C coupling at the solid-liquid interface

11:10am-12:00pm Seonah Kim: Computational Design Principles for Sustainable Chemistry

Wednesday, 19 July 2023

Session III: Electrochemical interfaces; Chairs: Greg Beran/John Keith

8:10am-9:00am Yue Qi: Complex Interfaces in Batteries

9:00am-9:50am Joerg Neugebauer: Electrochemistry in a periodic supercell

9:50am-10:20am Coffee Break

10:20am-11:10am Stefan Wippermann: Emerging concepts to simulate reactions at electrified interfaces

11:10am-12:00pm Ravishankar Sundararaman: Enhancing solvation models with MD and ML

Special evening session: Enzyme Catalysis; Chair: Yue Qi

7:30pm-8:20pm John Yang: Mutexa: A Predictive Modeling Platform for Enzyme Catalysis

Thursday, 20 July 2023

Session IV: Catalysis; Chairs: Wennie Wang/Ravishankar Sundararaman/Paul Zimmerman

8:10am-9:00am Michael Janik: Integrating DFT with classical FF MD to examine electrocatalytic systems

9:00am-9:50am Yuanyue Liu: Activation Energies of Heterogeneous Electrocatalysis

9:50am-10:20am Coffee Break

10:20am-11:10am Mira Todorova: Controlling doping of electrocatalysts through engineering impurities

11:10am-12:00pm Bill Schneider: Compositional Control and Catalysis in Ion-Exchanged Zeolites

Friday, 21 July 2021

Session V: Photo, chemical bonding, and transport; Chairs: Líney Árnadóttir/Bjork Hammer/Zach Ulissi

8:10am-9:00am Greg Beran: Design of organic photomechanical engines with exceptional work capacity

9:00am-9:50am Wennie Wang: Finding representative structural models in (photo)electrochemical systems

9:50am-10:20am Coffee Break

10:20am-11:10am John Keith: New Computational Tools for Exploring Chemical Bonding and Space

11:10am-12:00pm De-en Jiang: Molecular and ionic transport in novel materials

12:00pm – 12:15pm Concluding remarks; adjourn.