

2019 "Computational Materials Chemistry" Telluride Workshop
Venue: Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435
Tuesday morning, July 16, 2019 to Saturday noon, July 20, 2019; Breakfast starts 7:30am at School

Tuesday, 16 July 2019

8:20am-8:30am opening remarks

Session I: First Principles Electrochemistry and Implicit Solvation Models; Chair: De-en Jiang/Richard Hennig

8:30am-9:20am Minoru Otani, AIST, Japan: Development of the effective screening medium method

9:20am-10:10am Mira Todorova, MPIE, Düsseldorf: Ab initio approach to electrochemistry and corrosion

10:10am-10:40am Coffee Break

10:40am-11:30am Harald Oberhofer, Tech. Univ. Munich: Parametrizing Implicit Solvation Models

11:30am-12:20am Ravishankar Sundararaman, RPI: Grand-canonical continuum for FP electrochemistry

Wednesday, 17 July 2019

Session II: Electrocatalysis I; Chairs: Graeme Henkelman/Long Luo

8:30am-9:20am Yujie Sun, U. Cincinnati: Interfacing metals and compounds for enhanced hydrogen electrochemistry and organic transformations

9:20am-10:10am John Keith, U. Pittsburgh: Economical explorations of physical reaction mechanisms

10:10am-10:40am Coffee Break

10:40am-11:30am Andrew Peterson, Brown University: Understanding Pt's reactivity in HER

11:30am-12:20am Egill Skulason, U. Iceland: N₂ and CO₂ reduction reactions

6pm-8pm, Picnic at the school yard

8pm-9pm, Special evening session: Richard Hennig, U. Florida: Augmenting Machine Learning of Energy Landscapes with Local Structural Information

Thursday, 18 July 2019

Session III: Structure, Electronic Structure, and Energy Storage; Chairs: Harald Oberhofer/Mira Todorova

8:30am-9:20am Axel Gross, University of Ulm: Atomistic structures at electrode surfaces

9:20am-10:10am Yuanyue Liu: Electronic Structure Underlying Electrochemical Reactions of 2D Materials

10:10am-10:40am Coffee Break

10:40am-11:30am Kevin Leung, Sandia: Challenges in modeling battery interfaces

11:30am-12:20pm De-en Jiang, UC Riverside: Proton transport in electrode-confined water for pseudocap

Friday, 19 July 2019

Session IV: Electrocatalysis II; Chairs: Ravishankar Sundararaman/Minoru Otani

8:30am-9:20am Mike Janik, Penn state: DFT studies of electrocatalytic kinetics

9:20am-10:10am Karen Chan, DTU: How to determine electrochemical barriers and implications

10:10am-10:40am Coffee Break

10:40am-11:30am Long Luo, Wayne State: Gas Bubbles in Electrochemical Gas Evolution Reactions

11:30am-11:55am Jason Goodpaster, U. Minnesota: Magnetic and Electrocatalytic MOFs

11:55am-12:20pm Lei Li, UT Austin: Long timescale dynamics for catalysis

Saturday, 20 July 2019

Session V: Oxide Surfaces, Molten Salts, Flow Batteries, & Catalysis; Chairs: Axel Gross/Egill Skulason

8:30am-8:55am Chaitanya Kolluru, U. Florida: Role of magnetism on transitional metal oxide surfaces

8:55am-9:20am Lucas Koziol, ExxonMobil: Computing chemical reaction equilibria in molten salts

9:20am-9:55am Vitali Alexandrov, U. Nebraska: Electrochemistry of All-Vanadium Redox Flow Batteries

9:55am-10:25am Coffee Break

10:25am-10:50am Alexander Bagger, Univ. Copenhagen: Fingerprint of electrochemical interfaces

10:50am-11:15am Wenrui Chai, UT Austin: Isolated single Pt atom and few atom clusters for HER

11:15am-11:50am Hao Li, UT Austin: Catalytic Reactions at Alloy Surfaces