Workshop Program Schedule

07/24/2023 - 07/28/2023

Molecule Transformation through Proton-Coupled Electron Transfer for Energy Storage & Conversion

(<https://meetings.telluridescience.org/meetings/workshop-details?wid=1043>)

Organizers: Yuyan Shao, M.T.M. (Marc) Koper, Jenny Y. Yang

Telluride Intermediate School, 725 W Colorado Ave.

**Monday morning**

Presiders: M.T.M. (Marc) Koper, Jenny Yang

08:30-09:15 Jonas C. Peters (Caltech)

PCET as a strategy to mediate electrochemical and photoelectrochemical reductions while mitigating HER

9:15-10:00 Peter Strasser (TU- Berlin)

Exploring Chemical Selectivity of PCET

10:00-10:30 Break and discussion

10:30-11:15 Jillian L. Dempsey (UNC at Chapel Hill)

Kinetic Barriers to Metal Hydride Complex Formation in Fuel-forming Catalysis

11:15-12:00 Yogesh Surendranath (MIT)

Understanding interfacial hydride transfer reactions

**Monday afternoon**

Presider: Chong Liu

02:00-02:45 M.T.M. (Marc) Koper (Leiden Univ)

Cation-coupled electron transfer

02:45-03:30 Robert Warburton (Case Western Reserve Univ.)

First-Principles Modeling of Proton-Coupled Electron Transfer on Solid Surfaces

03:30-04:00 Discussion

**Tuesday morning**

Presiders: Jillian L. Dempsey, Charles McCrory

08:30-09:15 Jenny Yang (UC - Irvine)

Proton Transfer in CO2 Reduction and H2O Oxidation

0:15-10:00 Louise Berben (UC Davis)

Pre-equilibrium Reaction Mechanism and other Strategies to Enhance Rate and Lower Overpotential in Electrocatalysis

10:00-10:30 Break and discussion

10:30-11:15 Kara L. Bren (Univ. Rochester)

Roles of Endogenous and Exogenous Proton Transfers in Proton and Carbon Dioxide Reduction by Biomolecular Electrocatalysts

11:15-12:00 Marc Robert (Univ de Paris)

Multi PCET reactions to CO2 with molecular catalysts beyond 2 electrons and 2 protons

**Wednesday morning**

Presiders: Louise Berben, Yogesh Surendranath

08:30-09:15 Inke Siewert (Univ. Göttingen)

PCET for C=O reduction with molecules and materials

09:15-10:00 Charles McCrory (U. Michigan)

Considering the Role of Proton Transport in CO2 Reduction by Polymer-Encapsulated Cobalt Phthalocyanine

10:00-10:30 Break and discussion

10:30-11:15 Carlos Morales-Guio (UCLA)

Electrochemical CO2 Reduction Mechanism on Copper: Capturing Mesoscopic Transport and Intrinsic Kinetics

11:15-12:00 Karthish Manthiram (Caltech)

Controlling Interfacial Electron and Atom Transfer Reactions for Chemical Synthesis

**Wednesday afternoon**

Presiders: Robert Warburton

02:00-02:45 Yuyan Shao (Pacific Northwest National Lab)

Metal oxide proton relay in heterogenous electrocatalysis

02:45-03:30 Chong Liu (UCLA)

What and how can machine learning help towards mechanistic understanding in molecular electrochemistry

03:30-04:00 Discussion

**Thursday morning**

Presiders: Inke Siewert

8:30-9:15 Andrew Gewirth (UIUC)

Electrodeposited Metal, Alloy, and Composite Catalysts for CO2 and Methanol Electrocatalysis

9:15-10:00 Plamen Atanassov (UC Irvine)

Metal hydrides as catalysts for selective CO2 electro-reduction

10:00-10:30 Discussion