



Telluride Science Research Center Workshop

Molecular Chemistry in Electrochemical Energy Storage

When: July 09 – July 13, 2018

Where: Telluride Science Research Center, Telluride, CO

Organizers: T. Leo Liu (USU), Guihua Yu (UT, Austin), and Venkat Viswanathan (CMU)

Overview: TSRC workshops combine a small group setting, informal presentations, and in-depth discussions with afternoon hikes in the gorgeous Colorado mountains. This TSRC workshop focuses on mechanistic understanding and exploration of molecular chemistry in electrochemical energy storage including batteries, solar cells, electrolyzers, and supercapacitors. The primary task of the workshop is to invoke in-depth discussions on how electronic and steric factors, solvents, and additives affect electrochemical characteristics of organic and inorganic molecules in energy storage devices. It is anticipated that the workshop, at molecular level, will inspire creative solutions to existing challenges in current energy storage technologies, and spark novel ideas in developing new energy storage technologies.

Invited speakers by alphabetic order (last name):

Hye-Ryung Byon

(KAIST, Korea)

Zheng Chen

(UCSD, USA)

Jang-Wook Choi

(SNU, Korea)

Zhenxing Feng

(OSU, USA)

Brett Helms

(BNL, USA)

Kah Chun Lau

(CSU, USA)

Xianfeng Li

(DICP, China)

Karthish Manthiram

(MIT, USA)

Matt McDowell

(GIT, USA)

Robert Messinger

(CCNY, USA)

Joaquín Rodríguez-

López (UIUC, USA)

Kimberly See

(Caltech, USA)

Jennifer L. Schaefer

(UND, USA)

Jin Suntivich

(Cornell Uni.)

Yogi Surendranath

(MIT, USA)

Haotian Wang

(Harvard Uni, USA)

Qing Wang

(NUS, Singapore)

Xiaoliang Wei

(IUPUI, USA)

Qiang Zhang

(Tsinghua, China)

**TSRC Workshop: Molecular Chemistry
in Electrochemical Energy Storage
07/09/2018 - 07/13/2018**

Organizers: T. Leo Liu (Utah State University), Guihua Yu (UT-Austin), and Venkat Viswanathan (Carnegie Mellon University)

07/09 Monday, 7:45 am – 12:30 pm Materials and Interfacial Chemistry for Rechargeable Metal ion and Metal Batteries (I) (session chairs, Jang Wook Choi and Qiang Zhang)

7:45-8:30 Breakfast

1. 8:30-9:10 Li Metal Anode Protection in Safe Rechargeable Batteries (Qiang Zhang, Tsinghua University)
2. 9:10-9:50 Probing Interfacial Reactions in Energy Storage Devices Using Synchrotron X-ray Techniques (Zhenxing Feng, Oregon State University)
3. 9:50-10:30 Atomistic Simulation in Lithium-Sulfur Battery (Kah Chun Lau, California State University, Northridge)

10:30-10:50 Coffee break

4. 10:50-11:30 Molecular-Scale Understanding of Lithium & Aluminum Battery Materials Through NMR Spectroscopy: Local Disorder, Ion Dynamics, & Intercalation Mechanisms (Robert J. Messinger, The City College of New York)
5. 11:30-12:10 Supramolecular Chemistries for High Capacity Battery Electrode Binders (Jang Wook Choi, Seoul National University)

07/10 Tuesday, 7:45 am – 1:00 pm Materials and Interfacial Chemistry for Rechargeable Metal ion and Metal Batteries (II) (session chairs, Kim See and Matthew T. McDowell)

7:45-8:30 Breakfast

6. 8:30-9:10 Redox Organic Molecules for Stable and High Rate Li-ion Electrodes (Zhen Chen, University of California, San Diego)
7. 9:10-9:50 In Situ Investigation of the Dynamic Evolution of Materials and Interfaces in Batteries (Matthew T. McDowell, Georgia Institute of Technology)
8. 9:50-10:30 Computational Modeling of Next-generation Batteries for Electric Vehicles and Aviation (Venkat Viswanathan, Carnegie Mellon University)

10:30-10:50 Coffee break

9. 10:50-11:30 Employing Electrolyte Chemistry to Direct Processes in Next-Generation Batteries (Kim See, California Institute of Technology)
10. 11:30-12:10 Magnesium Electrolytes Based on Thermally Stable Solvents and Polymer Gels (Jennifer L. Schaefer, University of Notre Dame)
11. 12:10-12:40 Developing Mg-Sulfur Rechargeable Batteries through Electrolyte and Electrode Engineering (T. Leo Liu, Utah State University)

2:30-5:00 group activity (optional)

Hiking Jud Wiebe Trail (meet at the cross of N Aspen st. and W. Dakota Ave.)

07/11 Wednesday, 7:45 am – 1:30 pm Organic Materials for Redox flow batteries (session chairs, Qing Wang and Joaquín Rodríguez-López)

7:45-8:30 Breakfast

12. 8:30-9:10 Materials Development for Organic Redox Flow Batteries (Xiaoliang Wei, Indiana University-Purdue University Indianapolis)
13. 9:10-9:50 Redox-Active Polymer Electrolytes: New Solutions for Electrochemical Energy (Joaquín Rodríguez-López, University of Illinois Urbana-Champaign)
14. 9:50-10:30 Redox-Stable Cobalt-polypyridyl Complexes for Redox Flow Batteries (Hye Ryung Byon, Korea Advanced Institute of Science and Technology)

10:30-10:50 Coffee break

15. 10:30-11:10 The Marriage of Liquid and Solid Redox Chemistry: Redox-Targeting Based Energy Storage Systems from Concept to Reality (Qing Wang, National University of Singapore)
16. 11:30-12:10 Eutectic Solvent Electrolytes for High-Energy Cost-Effective Redox Flow Batteries (Guihua Yu, UT-Austin)
17. 12:10-12:50 Zinc Based Flow Battery for Stationary Energy Storage (Xianfeng Li, Dalian Institute of Chemical Physics)
18. 12:50-1:30 TBD (Brett Helms, BNL)

07/12 Wednesday 6:00-9:00 pm BBQ and Drinks at the meeting site (covered by the workshop)

07/12 Thursday, 7:45 am – 12:30 pm Electrocatalysis for Fuel Production (session chairs, Yogi Surendranath and Haotian Wang)

7:45-8:30 Breakfast

19. 8:30-9:10 Earth-abundant Transition Metal Electrocatalysts for Selective CO₂ Reduction in Water (Haotian Wang, Harvard University)
20. 9:10-9:50 Mechanism of Carbon Dioxide Reduction at Metal Macrocycles (Karthish Manthiram, MIT)

9:50-10:10 Coffee break

21. 10:10-10:40 Transition-Metal Oxide Catalysts Tailored at the Atomic Level: New Mechanistic Understanding and Design Implications (Jin Suntivich, Cornell University)
22. 10:40-11:10 Bridging Molecular and Heterogeneous Electrocatalysis Through Graphite Conjugation (Yogi Surendranath, MIT)

1:30-5:00 group activity (optional)

Hiking Bridal Veil Falls (meet at Idarado Mining, E Hwy 145 Spur)

<https://www.visittelluride.com/play/trails/>

07/12 Thursday 6:30-9:30 pm Workshop Dinner (covered by the workshop)

Sidework restaurant (225 S Pine St unit f, Telluride, CO 81435)

07/13 Friday 7:45-12:30 pm (optional)

7:45-8:30 Breakfast

8:30-12:30 Group discussions