

Workshop on Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion

August 5, 2024 - August 8, 2024

Telluride Depot 300 S Townsend St. Telluride, CO 81435

Organizers

| Veronica Augustyn | Associate Professor NC State University | vaugust@ncsu.edu |
|-------------------|--|---------------------------------|
| Anne Co | Professor Ohio State University | co@chemistry.ohio-state.edu |
| Don Siegel | Professor University of Texas at Austin | donald.siegel@austin.utexas.edu |
| Keith Stevenson | Professor and Consultant Watts kWh LLC | kjsaustin@msn.com |

Attendees

| Ilgar Baghishov | Postdoctoral Fellow University of Texas at Austin | baghishovilgar@austin.utex as.edu |
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| Véronique Balland | Professor Université Paris Cité | veronique.balland@paris7.j ussieu.fr |
| Bart Bartlett | Professor University of Michigan | bartmb@umich.edu |
| Ivano Eligio Castelli | Associate Professor Technical University of Denmark | ivca@dtu.dk |
| Nikita Dutta | Researcher National Renewable Energy Laboratory | Nikita.Dutta@nrel.gov |
| Matthew Gebbie | Assistant Professor University of Wisconsin | gebbie@wisc.edu |

| Samuel Greene | Postdoctoral Fellow University of Texas at Austin | samuel.greene@austin.utex as.edu |
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| Graeme Henkelman | Professor University of Texas at Austin | henkelman@utexas.edu |
| Yan-Yan Hu | Professor Florida State University | yhu@fsu.edu |
| Megan Jackson | Assistant Professor University of North Carolina, Chapel Hill | megan.jackson@unc.edu |
| Robert Kostecki | Senior Scientist Lawrence Berkeley National Lab | r_kostecki@lbl.gov |
| Joaquín Rodríguez-López | Professor University of Illinois at Urbana-Champaign | joaquinr@illinois.edu |
| Ellen Matson | Professor University of Rochester | ellen.matson@rochester.ed u |
| David Mitlin | Professor University of Texas at Austin | David.Mitlin@austin.utexas. edu |
| Rana Mohtadi | Toyota Research Institute of North America | rana.mohtadi@toyota.com |
| Yue Qi | Professor Brown University | YueQi@brown.edu |
| Srinivasan Ramakrishnan | Assistant Professor IIT Bombay | srini@chem.iitb.ac.in |
| Daniel Rettenwander | Professor Norwegian University of Science and Technology | daniel.rettenwander@ntnu.n o |
| Jaroslaw Syzdek | Product and Application Specialist Bio-Logic USA | jaroslaw.syzdek.apya@gma il.com |
| Yoshitaka Tateyama | Professor Tokyo Institute of Technology | tateyama.y.aa@m.titech.ac.j p |

Schedule

Breakfast served daily at 7:15 am at the Depot, 300 S. Townsend St. Lunch and dinner (except Wednesday) are on your own - self assemble into groups

Monday, Tuesday, and Thursday afternoons are open for group activities such as hiking, biking, and scientific discussion

| Day | Time | Event / Talk |
|----------------|--|--|
| Sunday 8/4 | 17 - 18:30 | Telluride Science Meet and Greet Alibi – 157 S. Fir Street This is a good chance to meet up with fellow participants before the meeting. A TSRC staff member will be on hand to welcome you and distribute badges. |
| Monday 8/5 | 7:15 - 8:20 8:20 - 8:30 8:30 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 | Breakfast (at the Depot) Opening Remarks Keith Stevenson, "Superconcentrated electrolytes: uncharted vs unchartered solutes" Matt Gebbie, "Exploring how ionic correlations influence interfacial electron transfer in electrochemical systems" Coffee Break Nikita Dutta, "Understanding Local Structures & Chemistry at Active Battery Interfaces with Operando Freezing Cryogenic Electron Microscopy" Yue Qi, "Modeling of the role of electric double layer (EDL) structures on SEI formation and the design of complex electrolytes" |
| | 18:30 - 19:20 19:20 - 19:55 19:55 - 20:20 | Rana Mohtadi, "Studies of interfacial behavior in metal anode batteries" Samuel Greene, "Computational Predictions of Ion Migration Barriers in Multivalent Solid Electrolytes from Phonon and Charge Density Features" Ilgar Baghishov, "Computational studies of Fe(III) Dihydroxybenzoquinone-Based Metal Organic Framework for Sodium Battery Cathodes" |
| Tuesday 8/6 | 7:15 - 8:30 8:30 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 | Breakfast Robert Kostecki, "New insights into the passivity of rechargeable battery electrodes in organic electrolytes" Megan Jackson, "Building a molecular graphite from the ground up" Coffee Break Joaquín Rodríguez-López, "Exploring the effects of electrostatics in interfacial electrochemistry: developing an analytical toolbox and venturing into emerging interfacial |

| | 11:30 - 12:20 18:30 - 19:30 | systems" Ellen Matson, Charge Compensation at the Surface of Polyoxovanadate-alkoxide Clusters Town Talk, Telluride Conference Center in Mountain Village Song Tan, Penn State University - "Chromatin: Your DNA in a package" |
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| Wednesday 8/7 | 7:15 - 8:30 8:30 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:20 - 1:20 | Breakfast Véronique Balland, "Solid-state charge carriers in aqueous batteries. A case study with TiO ₂ " Bart Bartlett, "How the Surface Chemistry of WO ₃ Influences its Activity for the Oxygen-Evolution- and Chloride Oxidation" Reactions Coffee Break Veronica Augustyn, "Solid state electrochemistry of protons" Anne Co, "Probing phase transitions and diffusion in electrodes" Catered lunch |
| | 13:20 - 14:10 14:10 - 14:40 14:40 - 15:30 17:30 - 19:30 | Yoshitaka Tateyama, "Microscopic electrochemistry for interface ionics based on DFT calculation" David Mitlin, "Grain Boundary Zirconia-Modified Garnet Solid-State Electrolyte" Ivano Castelli, "Towards an accelerated design of energy materials" TSRC Picnic at the Depot Free BBQ, beer, wine, and non-alcoholic beverages. Friends and family are invited free of charge. |
| Thursday 8/8 | 7:15 - 8:30 8:30 - 9:20 9:20 - 10:10 10:10 - 10:40 10:40 - 11:30 11:30 - 12:20 12:20 - 12:30 | Breakfast Daniel Rettenwander, "Enabling high conductive percolating networks in solid-state pouch cells" Yan Yan Hu, "Dendrite Formation at Interfaces in solid-state batteries probed with NMR and MRI" Coffee Break Srinivasan Ramakrishnan, "Designing Reactive Interphases for Anodeless Solid-State Batteries" Don Siegel, "Atomic Scale Modeling of "Anode Free" Li-Metal Batteries" Closing Remarks |