Telluride Science Research Center Workshop
"Structure and Function of the Hydrogenase Mimics"
Telluride Elementary School
447 West Columbia Avenue
June 29 – July 3, 2015

Sunday, June 28th	
6:00-8:00 PM:	**Informal gathering at Arroyo Wine Bar –** 220 E Colorado Ave., Telluride

Monday, June 29th Using Theory and Experiment to Understand the Hydrogenases	
7:30 AM	**Badge Pick-up and Breakfast**
8:00 AM	**Introduction**
8:15 AM	**John Peters –** "Structural aspects of hydrogenases and how insights were elucidated - what these enzymes do in nature"
9:00 AM	**Vincent Fourmond –** "Combining protein film voltammetry and theoretical chemistry to learn about the active site of hydrogenases"
9:45 AM	**Coffee Break**
10:15 AM	**Paul King –** "Proton-transfer and the catalytic cycle of [FeFe]-hydrogenase"
11:00 AM	**Martin Winkler –** "Substrate exchange and hydride formation in the catalytic mechanism of [FeFe]-hydrogenases"
11:45 AM	**Break for lunch in town**
1:30 PM	**Michael Hall –** "In Modeling Hydrogenases Computationally, Expect the Unexpected"
2:15 PM	**Simone Raugei –** "Toward Efficient Bio-inspired H2 Oxidation Catalysts: from Enzymatic Function to Functional Mimics"
3:00 PM	**Coffee Break**
3:15 PM	**Round Table (Michael Hall and John Peters)**
4:15 PM	**Adjourn**
6:30 PM	**Dinner in town (no host)**

Tuesday, June 30th Synthetic Studies Related to Understanding Hydrogenases	
7:30 AM	**Breakfast**
8:00 AM	**Marcetta Darensbourg –** "Expanding Landscapes of the Organometallic Molecules of Nature: inspirations from the Hydrogenase active sites and the molecules that are being built and transported by the maturases or precursor proteins"
8:45 AM	**Sascha Ott –** "MOFs as ways to mimic the protein matrix, and some unpublished work where we try to keep ligands "in place", avoiding rotational relaxation of kinetically formed terminal hydrides"
9:30 AM	**Coffee Break**
10:00 AM	**Monte Helm –** "Using theory to guide design – development of a bio-inspired Fe based hydrogen oxidation catalyst"
10:45 AM	**Chris Pickett –** "Aspects of Cyanide Chemistry in FeFe Subsite Analogues"
11:30 AM	**Break for lunch in town**
1:30 PM	**Morris Bullock –** "Using Proton Relays to Mimic the Function of the Hydrogenase Active Site"
2:15 PM	**Tom Rauchfuss –** "Review problems, failed attempts, and ongoing challenges with biomimetic catalysts"
3:00 PM	**Adjourn**
6:00 PM	**Telluride Town Talk –** Telluride Conference Center in Mountain Village
7:30 PM	**Cheese and Wine Round Table (Tom Rauchfuss and Marcetta Darensbourg) – Arroyo Wine Bar ($55/person)**

Wednesday, July 1st Mechanistic Studies Related to the Hydrogenases	
7:30 AM	**Breakfast**
8:00 AM	**Dennis Lichtenberger –** "Basic thermodynamics and kinetics of redox processes of hydrogenase mimics based on photoelectron spectroscopy, electrochemistry, and computations"
8:45 AM	**Leif Hammarström –** "Resolving catalytic intermediates with time-resolved spectroscopy (UV/VIS, IR)"
9:30 AM	**Coffee Break**
10:00 AM	**Eric Wiedner –** "Electrochemistry as a Mechanistic Tool: Applications to Nickel Diphosphine Electrocatalysts for Production of Hydrogen"
10:45 AM	**Anne Jones –** "Understanding and Controlling Bias of Hydrogenases"
11:30 AM	**Break for lunch in town**
1:30 PM	**Round Table (Eric Wiedner and Anne Jones)**
2:15 PM	**Adjourn (Group Hike – meet at the top of the Gondola at 2:45PM)**
6:00 PM	**TSRC Picnic/BBQ – Under the tent at the Elementary School**

Thursday, July 2nd Outer Coordination Sphere Studies to Understand the Function of Hydrogenases	
7:30 AM	**Breakfast**
8:00 AM	**Andy Borovik –** "Using Hydrogen Bonding and Protein Scaffolds to Control the Environment around Artificial Metal Enzymes"
8:45 AM	**Kara Bren –** "Cobalt Metalloprotein and Metallopeptide Electrocatalysts for Hydrogen Evolution from Water"
9:30 AM	**Coffee Break**
10:00 AM	**Molly O'Hagan –** "Using Catalyst Structural Dynamics to Maximize H2 Production Electrocatalysis"
10:45 AM	**Lisa Utschig –** "Photocatalytic hydrogen production from photosynthetic reaction center-molecular catalyst hybrids"
11:30 AM	**Break for lunch in town**
1:30 PM	**Hannah Shafaat –** "Hydrogen Production in Engineered Metalloprotein Scaffolds"
2:15 PM	**Wendy Shaw –** "Influence of the Outer Coordination Sphere on Catalytic Reactivity"
3:00 PM	**Adjourn**
7:00 PM	**Cheese and Wine Round Table (Wendy Shaw and Hannah Shafaat) – Location TBD**

Friday, July 3rd Conclusion Session	
7:30 AM	**Breakfast**
8:00 AM	**Akira Onoda –** "Artificial metalloenzyme and hybrid catalyst for various reactions/generating photocatalytic systems in which artificial metalloenzymes can be involved."
8:45 AM	**Manuela Gross –** "Nickel bisdiphosphine type complexes as catalysts for H2 generation in aqueous photo- and electrocatalytic systems"
9:30 AM	**Aaron Appel –** "Attaching molecular electrocatalysts to surfaces"
10:15 AM	**Final Round Table Discussion (Aaron Appel and Monte Helm)**
11:15 AM	**Closing Remarks/Adjourn Meeting**