# Telluride Science Research Center Workshop
# "Control of Proton and Electron Transfers in Redox Catalysis"
# Telluride Intermediate School
# 725 West Colorado Avenue
# August 7 – August 11, 2017

| Sunday, August 6th | |
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| **6:00-8:00 PM:** | **Informal gathering at the Phoenix Bean –** 221 W Colorado Ave., Telluride |

| Monday, August 7th | |
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| **7:30 AM** | **Badge Pick-up and Breakfast** |
| **8:00 AM** | **Introduction** |
| **8:15 AM** | **Oliver Lenz –** "Redox catalysis by [NiFe]-$H_2$ase: the importance of having both a catalytic and an electron-transferring subunit." |
| **9:00 AM** | **Anne Jones –** "Defining functional diversity of $H_2$ase electrochemically" |
| **9:45 AM** | **Coffee Break** |
| **10:15 AM** | **Christophe Leger –** "Combining electrochemistry and theoretical calculations to learn about the reaction of [FeFe]-$H_2$ase with inhibitors: CO, $O_2$ and light." |
| **11:00 AM** | **Olaf Ruediger –** "Why $H_2$ases operate at low overpotential?" |
| **11:45 AM** | **Break for lunch in town** |
| **1:30 PM** | **Arnub Dutta –** "Reversibility in Molecular Complexes Requires Components from Enzymes" |
| **2:15 PM** | **Nicholas Plumere –** "Reversible electron transfer for reversible $H_2$ase catalysis in redox matrices" |
| **3:00 PM** | **Greg Schenter –** "Protein bath: what is more important, electrostatics or molecular orbitals" |
| **3:45 PM** | **Adjourn** |
| **6:30 PM** | **Dinner in town** |

| Tuesday, August 8th | |
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| **7:30 AM** | **Breakfast** |
| **8:00 AM** | **Frank Sargent –** "The formate hydrogenlyase complex: enclosed electron transfer between molybdenum and nickel" |
| **8:45 AM** | **Zachariah Heiden –** "PCET reactions promoted by fluorescent dye molecules" |
| **9:30 AM** | **Coffee Break** |
| **10:00 AM** | **Jenny Yang –** "New ligand platforms to orchestrate proton/electron transfer" |
| **10:45 AM** | **Sean Elliott –** "Proton coupling and catalysis in the hydrogen dependent $CO_2$ reductase of *A. woodii*" |
| **11:30 AM** | **Break for lunch in town** |
| **1:30 PM** | **Louise Berben –** "Selective C-H bond formation with $CO_2$: mechanistic insights with molecular electrocatalysts" |
| **2:15 PM** | **Jim Mayer –** "Oxidizing O–H and C–H bonds by concerted but separated proton/electron transfers" |
| **3:00 PM** | **Adjourn** |
| **6:00 PM** | **Telluride Town Talk –** Telluride Conference Center in Mountain Village |
| **7:30 PM** | **Round Table – Location TBD** |

| Wednesday, August 9th | |
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| **7:30 AM** | **Breakfast** |
| **8:00 AM** | **Marcetta Darensbourg –** "Developing a matrix of heterobimetallic complexes for interrogation of hydrogen evolution reaction electrocatalyts" |
| **8:45 AM** | **Mike Hall –** Computational modeling of structures and mechanisms for hydrogen oxidation and production on transition-metal complexes |
| **9:30 AM** | **Coffee Break** |
| **10:00 AM** | **Paul King –** "Photochemically driven mechanistic studies of redox enzymes" |
| **10:45 PM** | **Martin Winkler –** "Probing transient H-cluster states and unresolved IR-spectroscopic features of [FeFe]-$H_2$ase" |
| **11:30 PM** | **Break for Lunch in town** |
| **1:30 PM** | **Molly O'Hagan –** "Mimicking the functions of protein scaffolds in catalysts for $H_2$ production and oxidation" |
| **2:15 PM** | **Hannah Shafaat –** "Towards a mechanistic understanding of catalytic hydrogen production by nickel-substituted rubredoxin" |
| **3:00 PM** | **Yi Lu –** "Understanding heteronuclear metalloenzymes involved in multi-electron and multi-proton processes through protein design" |
| **3:45 PM** | **Adjourn** |
| **6:00 PM** | **TSRC Picnic/BBQ – Under the tent at the Elementary School** |

| Thursday, August 10th | |
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| **7:30 AM** | **Breakfast** |
| **8:00 AM** | **Lance Seefeldt –** "Insights into the nitrogenase mechanism" |
| **8:45 AM** | **Bojana Ginovska –** "Mechanistic insight in key steps of $N_2$ reduction by nitrogenase: a computational study" |
| **9:30 AM** | **Coffee Break** |
| **10:00 AM** | **Yashiro Ohki –** "Bio-inspired transition metal cluster molecules: synthesis and application in $N_2$ transformation" |
| **10:45 AM** | **Kyle Lancaster –** "Hydroxylamine oxidation at Heme P460 Centers: fuel vs futility" |
| **11:30 AM** | **Nate Szymcsak –** "Moving beyond the metal: assisted small molecule activation" |
| **12:15 PM** | **Break for lunch in town** |
| **2:15 PM** | **Group Activity** |
| **7:00 PM** | **Social – Location TBD** |

| Friday, August 11th Conclusion Session | |
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| **7:30 AM** | **Breakfast** |
| **8:00 AM** | **Russ Hille** – "A Trip Down Memory Lane: electron transfer in complex flavoproteins" |
| **8:45 AM** | **John Peters –** "Mechanisms of electron bifurcation" |
| **9:30 AM** | **David Beratan –** "The thermodynamics and kinetics of electron bifurcation" |
| **10:15 AM** | **Closing Remarks/Adjourn Meeting** |
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