## Telluride Workshop on Proton Transfer in Biology, July 16-20<sup>th</sup> 2024

## **Telluride Intermediate School**

725 W Colorado Avenue

Organizers: Joachim Heberle, Brian Dyer, and Jessica Swanson Local TSRC Host: Mark Kozak (970-708-4426)

July 15 <sup>th</sup> Monday			
5:00-6:30 (pm)	All-Telluride Science Meet and Greet Location: <u>Alibi</u> (157 S. Fir Street, Telluride) * there will be drinks and badges – hope to see you there!		
July 16 <sup>th</sup> Tuesday	Discussion Leader: Jessica & Brian		
7:30-8:00 (am)	Registration & "Grab & Go" Breakfast in coffee break area		
8:00-8:10	Introduction Mark Kozak, TSRC Director + Organizers		
8:10-8:50	Brian Dyer Proton coupled electron transfer i	Emory University n hydrogenases	
8:50-9:30	Katherine White Spatiotemporal pH dynamics in bi	University of Notre Dame ology: New tools and molecular insights	
9:30-10:10	Katie Henzler-Wildman University of Wisconsin - Madison Proton coupling versus proton leak in the Small Multidrug Resistance transporters		
10:10-10:40	Coffee Break		
10:40-11:20	Rob Burnap Coupling CO <sub>2</sub> hydration with cyclic NDH-1 complexes in cyanobacteri	Oklahoma State c photosynthetic electron flow via specialized a	
11:20-12:00	Jessica Swanson Unraveling the Role of Kinetic Sele	University of Utah ection in Channels and Transporters	
12:00-12:40	Robert B Gennis University of Illinois  Structure and Mechanism of the Energy-coupled Transhydrogenase from E. coli		
2:30-4:30 (pm)	Hike to the oxidase waterfall in honor of Mårten Wikström		
6:30-7:30 (pm)	Town Talk (Telluride Conference Center, 580 Mountain Village Blvd, Mountain Village, CO 81435) Cash bar starts at 6:00pm Title: Methane: Supercharging Nature's Solution to Reverse Climate Change Speaker: Jessica Swanson		

Moderators: Judy Muller (ABC) & George Lewis (NBC)

July 17 <sup>th</sup> Wednesday	Discussion Leader: Huong Kratochvil		
7:30-8:00 (am)	Breakfast (Telluride Intermediate School)		
8:00-8:40	Ramona Schlesinger Charge transfer in the heterologic kHV1 from Karlodinium veneficu	Freie Universität, Berlin ously expressed voltage-gated proton channel m	
8:40-9:20	Helmut Grubmüller Max Planck Institute for Multidisciplinary Sciences Solvation shell thermodynamics and constant pH simulations with FMM electrostatics		
9:20-10:00	Greg Voth  Multiscale Simulation and Kinetic Systems	University of Chicago c Modeling of Proton Transport in Biomolecular	
10:00-10:30	Coffee Break		
10:30-11:10	Sylvie Roke Imaging / spectroscopy experime interfaces	EPFL ents on protons in water at membrane	
11:10-11:50		Stockholm University ransfer mechanisms in complex bioenergetic	
11:50-12:30	Marilyn Gunner Following the protons in complex	City College of New York  I using MCCE microstate analysis	
5:30-7:30 (pm)	All Telluride Science Picnic Free BBQ, Beer, Wine, and Non-Alcoholic Beverages. Friends and Family are invited free of charge. Location: Tent behind the Intermediate School		
July 18 <sup>th</sup> Thursday	Discussion Leader: Ville Kaila		
7:30-8:00 (am)	Breakfast (Telluride Intermediate School)		
8:00-8:40	Noam Agmon Cation and proton diffusion at th	The Hebrew University of Jerusalem e membrane water interface	
8:40-9:20	Ana-Nicoleta Bondar  Conserved hydrogen-bonding an of membrane receptors and tran	University of Bucharest d hydrophobic interaction networks in families sporters	
9:20-10:00	Kalina Hristova	Johns Hopkins University	

	Bias in transmembrane signal transduction by single pass receptors		
10:00-10:30	Coffee Break		
10:30-11:10	Gustav Beggren Exploring proton transfer in hydrohydrogenase diversity	Uppsala University ogen catalysis – lesson learned from [FeFe]	
11:10-11:50	Huong Kratochvil  Proton transport mechanism thro	University of North Carolina at Chapel Hill ough the lens of de novo protein design	
11:50-12:30	William Wimley Structural Determinants of pH-re	Tulane University School of Medicine sponsive Peptide Nanopores	
July 19 <sup>th</sup> Friday	Discussion Leader: Kalina Hristova		
7:30-8:00	Breakfast (Telluride Intermediate School)		
8:00-8:40	Petra Hellwig  Reactivity of oxygen reducing enviolential spectroscopies	University of Strasbourg zymes, insights from electrocatalysis and	
8:40-9:20	Boris Musset Mutations in the Voltage-Gated I	PMU Nuremberg Proton Channel Raise New Questions	
9:20-10:00	Ruibin Liang Texas Tech University  Understanding the Multifaceted Mechanism of Compound I Formation and Reactivity in Unspecific Peroxygenases through Multiscale Simulations		
10:00-10:30	Coffee Break		
10:30-11:10	Keiichi Inoue Proton Transfer in Ion-transportii	The University of Tokyo ng Microbial Rhodopsin	
11:10-11:50	Joachim Heberle Proton transfer in LOV domains	Freie Universität, Berlin	
11:50-12:30	General Discussion/Meeting Wrap Up (Planning for 2026)		
July 20 <sup>th</sup> Saturday	Hiking, Departure		