

Water: Grand Challenges for Molecular Science and Engineering

Organizers: Seth Darling and Giulia Galli

Location: Telluride Intermediate School, 725 W Colorado Ave, Telluride, CO 81435



Telluride Science Research Center

	Saturday 6/15	Sunday 6/16	Monday 6/17	Tuesday 6/18	Wednesday 6/19	Thursday 6/20
8:30-9:00		Free time	Breakfast	Breakfast	Breakfast	Breakfast
9:00-9:45			F Gygi <small>Structural and electronic properties of water from DFT meta-GGA first principles MD simulations</small>	J Skinner <small>Anomalies in ambient and supercooled water: Is there a second critical point lurking nearby?</small>	T Li <small>Anomalous stability of interfacial ice revealed by freezing of water in confinement</small>	A Noy <small>Ion transport in carbon nanotube porins: Confinement, correlation, and coupling effects</small>
9:45-10:30			N Levinger	A Nilsson <small>X-ray studies of water from hot to deep supercooled conditions</small>	V Molinero <small>Molecular modeling of anion exchange membranes for fuel cells</small>	R Car
10:30-11:00			Break	Break	Break	G Galli <small>First principles simulations of water at oxides and semiconductors interfaces</small>
11:00-11:45			M Fernández-Serra <small>Ab initio modeling of anion-cation association in water: unravelling the effects of sampling, water structure and charge localization in structure and dynamics of ion pairs</small>	W Phillip <small>Expanding the Functionality of Membranes for Water Treatment Through Additive Manufacturing</small>	A Selloni <small>Structure, dynamics and polarization of interfacial water on titania</small>	Wrap-up discussion
11:45-12:30			J Chen <small>Real-time Detection and Selective Removal of Lead Ions in Drinking Water</small>	B Freeman <small>Ion Sorption, Diffusion and Transport in Charged Polymer Membranes</small>	C Fennell <small>Some Potential in Pairwise Water Potentials</small>	
12:30-2:00			Lunch break (on your own)	Free time	Lunch break (catered at TSRC, courtesy UChicago)	
2:00-2:45			F Paesani <small>Towards a realistic modeling of hydration, one molecule at a time</small>		C Stafford <small>Structure and dynamics in polyamide-based desalination membranes</small>	
2:45-3:30			T Pham <small>Nanoscale solvation from Ab-Initio Simulations</small>		C Osuji <small>Nanoporous membranes from self-assembled materials: Progress towards the promise</small>	
3:30-4:00			Break		Break	
4:00-4:45			B Winter <small>Nanoparticle-aqueous solution interface studied by liquid-jet photoemission</small>		S Ardo <small>Fundamental studies of water as a protonic semiconductor: consequences for ionic solar cells</small>	
4:45-5:30			F Perakis <small>Crystallite formation and brine rejection in NaCl aqueous solutions</small>		N Aluru <small>Water in solid oxides</small>	
6:00-6:15	Registration (6-8 PM at the Phoenix Bean)	Welcome		Town Talk at Telluride Conference Center in Mountain Village (6:30-7:30 PM)	TSRC Picnic (open to family/friends)	
6:15-7:00		S Darling <small>Water technologies by interface engineering</small>				
7:00-7:45		A Packman <small>Ubiquitous anomalous processes resulting from fluid interactions with complex surfaces and pore structures</small>	Workshop dinner (Sideworks)			
7:45-8:30		V John <small>Oil Spills, Oil Recovery, and the Red Tide – a unifying approach to these water challenges</small>				