

**Hydrophobicity: From Theory, Simulation, to Experiment, July 12 – 16, 2016**

Telluride Elementary School, 447 West Columbia Ave Telluride, CO 81435

**Monday, July 11, 2016, 6:00 – 8:00 pm** Reception and early badge pick-up at the tent outside the Elementary School. Complimentary beer and wine will be provided.

**Tuesday, July 12, 2016 (8 talks)**

Morning Session (8:30 am – 12:30 pm)

*Hydrophobically Driven Assembly*

**8:30 – 8:45** Introductory Remarks

**8:45 – 9:30 Gregor Weiss:** Kinetic design of hydrophobic key-lock association: Pocket geometry and physicochemical properties

**9:30 – 10:30 Pratyush Tiwary:** The role of water in the kinetics of ligand unbinding

15 min break

**10:45 – 11:30 Kenji Mochizuki:** Influence of co-nonsolvency on the aggregation of tertiary butyl alcohol in methanol-water mixtures

**11:30 – 12:30 Hank Ashbaugh:** Cavitands and Alkanes: Some Assembly Required

Afternoon Session (2:15 – 4:00 pm)

*Designing Novel Materials*

**2:15 – 3:15 Alenka Luzar:** Superhydrophobicity, Janus interfaces, curved hydrophobes

**3:15 – 4:00 Arun Kota:** Super-Repellent Surfaces: Design and Applications

Evening Session (6:30 – 8:30 pm)

*Protein Hydrophobicity, Interactions, and Aggregation*

**6:30 – 7:30 Amish Patel:** Hydration at Nanostructured Surfaces: Applications to Protein Interaction Prediction and Materials Design

**7:30 – 8:30 Peter Vekilov:** Hydrophobicity enables the nucleation precursors in protein aggregation

**Wednesday, July 13, 2016 (6 talks)**

Morning Session (9 am – noon)

*Macromolecules and Ions*

**9:00 – 10:00 Paul Cremer:** Do neutral polymers attract hydronium or hydroxide?

**10:00 – 11:00 Andrew Ferguson:** Nonlinear reconstruction of hydrophobic folding funnels from experimentally measurable time series

**11:00 – noon Dongmao Zhang:** Ion pairing and recombination: Solvent-dependent Organothiol Binding to Gold

Afternoon Session (2:15 – 5:00 pm)

*Fundamentals of Hydrophobicity – Theory and Computation*

**2:15 – 3:15 John Weeks:** Local Molecular Field theory for effects of solute attractive forces on hydrophobic solvation and association

**3:15 – 4:00 Mangesh Chaudhari:** Statistical analyses of hydrophobic interactions

**4:00 – 5:00 Ali Hassanali:** Holes in Water and other hydrophobic effects

Evening PICNIC (6 pm – 9 pm)

**Thursday, July 14, 2016 (6 talks)**

Morning Session (9:00 am – noon)

*Solvation at Interfaces*

**9:00 – 10:00 Ken Koga:** The solubility of nonpolar solutes at the liquid-vapor interface of water: A simple mean-field description

**10:00 – 11:00 Eric Tyrode:** Water and Ions at extended solid/liquid hydrophobic interfaces as revealed by vibrational sum frequency spectroscopy

**11:00 – noon Barbara Wyslouzil:** Co-condensation of immiscible compounds: Particle formation & structure

Afternoon FREE

Evening Session (6 – 9 pm)

*Co-solutes and Co-solvents*

**6:00 – 7:00 Nico van der Vegt:** Solvation at the air-water interface OR Cosolvent effects on the hydrophobic polymer collapse transition

**7:00 – 8:00 Gren Patey:** Aqueous t-Butanol (TBA) Solutions Revisited

**8:00 – 9:00 Guillaume Stirnemann:** On the protective osmolyte effect of TMAO on polymer chains and on its influence on water dynamics as compared to that of extended hydrophobic interfaces

**Friday, July 15, 2016** (7 talks)

Morning      Session      (9 – 11:30 am)

*Hydrophobicity in Biology*

**9:00 – 10:00 Monte Pettitt:** Peptide aggregation: hydrophobicity vs solubility

**10:00 – 11:00 Stephen White:** The hydrophobic effect in membrane protein folding

**11:00 – 11:30 Emiliano Brini:** TBA

Afternoon      Session      (2 – 6:00 pm)

*Fundamentals of Hydrophobicity – Experiments*

**2:00 – 3:00 Haitao Liu:** On the intrinsic wettability of graphitic carbon

**3:00 – 4:00 Sylvie Roke:** Hydrophobic / water interfaces

15 min break

**4:15 – 5:00 E-Jen Teh:** New surfaces for hydrophobic force measurements

**5:00 – 6:00 Dor Ben-Amotz:** Water-mediated hydrophobic interactions: experiments vs theory

Evening      FREE

**Saturday, July 16, 2016**      FREE TIME