

Hydrophobicity: From Theory, Simulation, to Experiment, June 26 – 30, 2022
Telluride Intermediate School, 725 West Colorado Ave Telluride, CO 81435

Saturday, June 25, 2022

5:00 – 6:30pm **TSRC Meet & Greet** at Phoenix Bean, 221 W Colorado Ave

6:00 – 8:00 pm **Social Gathering** at High Pie Pizzeria on Colorado Ave at Pine St

Sunday, June 26, 2022

8:00 – 9:00 am Breakfast (at Telluride Intermediate School)

9:20 am **Group Hike**, meet at Bear Creek trailhead on S. Pine Street

1:00 – 1:05 pm **Introductory Remarks**

1:05 – 2:30 pm **Perspective Discussion**

Participants to present grand challenge/vision driving their research & ways this group can help.
All participants will present for 2 mins with 3 mins for discussion (*no more than 1-2 slides*).

2:30 – 3:00 pm Break

Biomolecular Hydration

3:00 – 4:00 pm **Jeremy Smith**, ORNL/U Tennessee
“Hydration at Biomolecular Surfaces. What does it control?”

4:00 – 4:15 pm Break

4:15 – 5:15 pm **Rachel Martin**, UC Irvine
“Clear as crystallin: the role of hydrophobic hydration in the human eye lens”

5:15 – 5:30 pm Break

5:30 – 6:30 pm **Gul Zerze**, U Houston
“Atomistic Simulations of RNA Folding in Bulk Aqueous Solutions and under Confinement”

Monday, June 27, 2022

8:00 – 9:00 am Breakfast

Water-Mediated Interactions

9:00 – 10:00 am **Amish Patel**, U Penn
“Context-Dependence of Hydrophobicity and Hydrophobic Interactions”

10:00 – 10:15 am Break

10:15 – 11:15 am **Adam Urbach**, Trinity U
“Cucurbituril-Peptide Interactions in Aqueous Solution”

11:15 – 11:30 am Break

11:30 am – 12:30 pm **Scott Shell**, UCSB
“Inverse design of water-mediated interactions”

12:30 pm – 2:30 pm Break for Lunch

Fundamental Understanding of Hydrophobic Effects

2:30 – 3:30 pm **Sumit Sharma**, Ohio U
“Hydration of linear alkanes is governed by the small length-scale hydrophobic effect”

3:30 – 3:45 pm Break

3:45 – 4:45 pm **Martina Havenith**, Ruhr U Bochum
“Spectroscopic Fingerprints of Cavity Formation and Solute Insertion as a Measure of Hydration Entropic Loss and Enthalpic Gain”

4:45 – 5:00 pm Break

5:00 – 6:00 pm **Hank Ashbaugh**, Tulane
“Fluctuations and Hydrophobic Effects”

Tuesday, June 28, 2022

8:00 – 9:00 am Breakfast

Hydrophobically-Driven Assembly

9:00 – 10:00 am **Dor Ben-Amotz**, Purdue
“Influence of ions on neutral surfactant micelle formation”

10:00 – 10:15 am Break

10:15 – 11:15 am **Matej Kanduc**, Jozef Stefan Institute, Ljubljana
“Monolayer Adsorption Versus Bulk Micellization: Insight from Molecular Simulations”

11:15 – 11:30 am Break

11:30 am – 12:30 pm **Bruce Gibb**, Tulane
“Solvation of, and guest binding mechanisms to, non-polar pockets”

Afternoon **Free Time**

6:30 – 7:30 pm **Town Talk**, Telluride Transfer Warehouse (201 S Fir Street)
Speakers: Moh El-Naggar, Ron Naaman, and Dave Waldeck
<https://www.telluridescience.org/for-the-public/2022-town-talk-calendar>

Wednesday, June 29, 2022

8:00 – 9:00 am Breakfast

Ions and Hydrophobicity

9:00 – 10:00 am **Werner Nau**, Jacobs U
“Superchaotropic Anions”

10:00 – 10:15 am Break

10:15 – 11:15 am **Ken Koga**, Okayama U
“Osmotic second virial coefficients for hydrophobic interactions: Ion-specific effects and solute-size dependences”

11:15 – 11:30 am Break

11:30 am – 12:30 pm **Paul Cremer**, Penn. State
“Partitioning Salt Ions Away from Polymer/Water Interfaces”

12:30 pm – 3:00 pm Break for Lunch

3:00 – 5:30 pm **Retrospective Discussion** (format to-be-determined)
What are the grand challenges? What is the state-of-the-art? Where are the knowledge gaps?
Where are the exciting opportunities: synthesis, characterization, algorithms, machine learning?
Which problems demand synergistic interactions between researchers with disparate toolkits?

5:30 – 5:45 pm **Concluding Remarks**

5:30 – 7:30 pm **TSRC Picnic** in Tent behind Telluride Science Workshop Facility
725 W Colorado Ave

Thursday, June 30, 2022

8:00 – 9:00 am Breakfast

Free time