

Hybrid Program: For both Virtual and On Site Participants

A google document shared with all participants will be kept running throughout the conference. People will each have a table in which under each person they can write questions that came up or points that were raised during either the virtual meetings or walks in beautiful Telluride. This way everyone can feel or be part of the collective discussion.

Timings MST	June 11th	June 12th	June 13th	June 14th	June 15th
Chairs	Sylvie Roke+ Ali Hassanali	Richard Remsing + Ana Vila Verde	Nancy Levinger + Elise Duboué-Dijon	David Wilkins+ Gul Zerze	Matthias Heyden + Huib Bakker
8:15-8.45	Welcome and introduction	Ali Hassanali (V)	Dor Ben-Amotz	Paul Cremer	Nancy Levinger
8:45-8:55	Break	Break and discuss	Break and discuss	Break and discuss	Break and discuss
8.55-9.25	Matthias Heyden	Elise Duboué-Dijon (V)	Gabriele Sosso (V)	David Wilkins	Feng Wang
9:25-9.55	Joint Discussions	Joint Discussions	Joint Discussions	Joint Discussions	Joint Discussions
9.55-10.25	Jene Cyran	Biman Bagchi (V)	Sylvie Roke	Ana Vila Verde (V)	Gul Zerze (V)
10:25-10:35	Break and discuss	Break and discuss	Break and discuss	Break and discuss	Break and discuss
10.35-11.05	Richard Remsing	Huib Bakker (V)	Mark Berg	Thomas Kuhne (V)	Zahra Fakhrai (V)
11.05-12.00	Joint Discussions	Joint Discussions	Joint Discussions	Joint Discussions	Closing Remarks

Titles of Talks:

1. Matthias Heyden: "Solvation Free Energy Arithmetics: Building Solvation Models One Functional Group at a Time"
2. Jene Cryan: "Molecular Insights to Ice Nucleation Abilities of Perfluorooctanoic Acid"
3. Richard Remsing: "Defects and Excess Electrons at Semiconductor-Liquid Interfaces"
4. Ali Hassanali: "Unsupervised Learning of the Structure and Dynamics of Liquid Water"
5. Elise Duboué-Dijon: "Ion binding to biomolecules, should we trust simulations? What can we really learn from them?"
6. Nancy Levinger: "Nanoconfinement impacts on/of urea in/on reverse micelles"
7. Huib Bakker: "Effect of ions and surfactants on the properties of interfacial water"
8. Dor Ben-Amotz: "Interfacial adsorption of ions in water droplets"
9. Gabriele Sosso: "The Formation of Ice at Biological Interfaces: a Computational Perspective"
10. Sylvie Roke: "Hydrophobicity and Confinement"
11. Mark Berg: "Micelle Dynamics Using MUPPETS: An Example of Multidimensional Kinetics"
12. Paul Cremer: "Cation Specific Binding to Monolayers of Oxyanions"
13. David Wilkins: "Symmetry-Adapted Machine Learning and Vibrational Spectroscopy"
14. Ana Vila Verde: "Quantifying C-F...water interactions"
15. Thomas Kuhne: "Timbling with a limb: Local asymmetry of water's hydrogen bond network and its consequence"
16. Biman Bagchi: "Nanoconfined water and its anomalies: Search for a length scale"
17. Feng Wang: "Surface Exclusion, Penetration, and Enrichment of Simple Ions from MP2 based simulations"
18. Gul Zerze: "Atomistic Simulations of RNA Folding in Bulk Aqueous Solutions and under Confinement"
19. Zahra Fakhrai: "Understanding the role of entropy in dynamics in confinement"

Program for Virtual Participants:

Short presentations (20 mins from each speaker discussing open problems/areas that each person is working on. Focus on unpublished work and different topics from what will be discussed in the main meeting.

Timings CET	June 11th	June 12th	June 13th	June 14th
3 PM -4.00 PM CET	<u>TBA</u>	<u>TBA</u>	<u>TBA</u>	<u>TBA</u>

Program for In-Person Participants:

Short presentations (20 mins from each speaker discussing open problems/areas that each person is working on. Focus on unpublished work and different topics from what will be discussed in the main meeting.

Timings MST	June 11th	June 12th	June 13th	June 14th