

Interfacial Molecular and Electronic Structure and Dynamics

Monday July 2 to Friday July 6

Monday Morning (8:30am-12:00 noon) Session: *Ions and Ionic Liquids*

7:30-8:30 Breakfast at the School

8:30-8:45 Introductory Remarks: Dor Ben-Amotz and Nana

8:45-9:15 **Marcel Baer** "Bulk and interfacial solvation of monatomic and polyatomic anions/acids using DFT"

9:15-9:30 *Discussion*

9:30-10:00 **Steven Corcelli** "Solvation Dynamics in Ionic Liquids"

10:00-10:15 *Discussion*

10:15-10:30 Break

10:30 -11:00 **Liem Dang**, "Computational studies of aqueous and ionic liquids interfaces"

11:00-11:15 *Discussion*

11:15 -11:45 **Theresa Head-Gordon**, "TBA"

11:45-12:00 *Discussion*

Monday Evening (7:00 pm – 9:15 pm) Session: *Air-Water Interface*

7:00-7:30 **Agustin Colussi**, "Recent experimental results on the two sides and many dimensions of the air-water interface"

7:30 -7:45 *Discussion*

7:45-8:15 **Revati Kumar**, "The hydroxide ion at the air-water interface"

8:15 -8:30 *Discussion*

8:30-9:00 **Steven Rick**, "Charge transfer interactions at interfaces"

9:00 -9:15 *Discussion*

Tuesday Morning (8:45am-12:00 noon) Session: *Molecular Interfaces*

7:30-8:45 Breakfast at the School

8:45-9:15 **Dor Ben-Amotz**, "Interactions Between Halide Anions and a Molecular Hydrophobic Interface"

9:15-9:30 *Discussion*

9:30-10:00 **Mike Hands**, "Modeling Aqueous Solutions Using the Effective Fragment Potential Method"

10:00-10:15 *Discussion*

10:15-10:30 Break

10:30 -11:00 **Paul Cremer**, "Positively Charged, Negatively Charged, and Hydrophobic/Aqueous Interfaces with Added Salt: An SFG Study"

11:00-11:15 *Discussion*

11:15 -11:45 **Peter Rossky**, "Charge separation at organic molecular interfaces"

11:45-12:00 *Discussion*

Tuesday Afternoon (2:00pm - 5:15pm) Session: ***Biological Interfaces***
2:00-2:30 ***Kelly Gaffney***, “Ligand Exchange and Ion Assembly in Polar Solvents: Mechanisms and dynamics”
2:30-2:45 *Discussion*
2:45-3:15 ***Amber Krummel***, “Exploring Surfactin-Lipid Interactions with IR Spectroscopy”
3:15 -3:30 *Discussion*
3:30-3:45 Break
3:45-4:15 ***David Leitner***, “Dynamics of water at the interface between proteins”
4:15-4:30 *Discussion*
4:30 -5:00 ***Dmitry Matyushov***, “Liquid dielectric response of a nanometer interface”
5:00-5:15 *Discussion*

Tuesday Evening (6:00-7:15)
Town Talk at the Palm Theatre

Wednesday Morning (8:45am-12:00 noon) Session: ***Nano-Interfaces & Confinement***

7:30-8:45 Breakfast at the School
8:45-9:15 ***Thomas Klar***, “Nano-local observation of adsorption of anions using single gold nanoparticle spectroscopy”
9:15-9:30 *Discussion*
9:30-10:00 ***Branka Ladanyi***, “Structure and dynamics of nanoconfined water”
10:00-10:15 *Discussion*
10:15-10:30 Break
10:30 -11:00 ***Aaron Lindenberg***, “Ultrafast structural dynamics in nanocrystals and in thin films probed by ultrafast x-ray and THz spectroscopy”
11:00-11:15 *Discussion*
11:15 -11:45 ***Sylvie Roke***, “Water structure @ nanodroplet interfaces”
11:45-12:00 *Discussion*

Wednesday Evening (7:00 pm – 9:15 pm) Session: ***Nano-Interfaces & Confinement***
7:00-7:30 ***Michael Tauber***, “Singlet fission in carotenoid nanoparticles”
7:30 -7:45 *Discussion*
7:45-8:15 ***Alberto Striolo***, “Hydrodynamic Slip as Predicted by Static and Dynamic Contact Angles, and Effect of Water Orientation at Graphene Interfaces on Performance of Electric Double Layer Capacitors”
8:15 -8:30 *Discussion*
8:30-9:00 ***Ward Thompson***, “Reorientational and Hydrogen-Bond Dynamics in Nanoconfined Liquids”
9:00 -9:15 *Discussion*

Thursday Morning (8:45am-12:00 noon) Session: *Hydrated Electrons*
7:30-8:45 Breakfast at the School
8:45-9:15 **Laszlo Turi**, “Quantum Dynamics Simulations on the Lifetime of Excited State Water Cluster Anions”
9:15-9:30 *Discussion*
9:30-10:00 **John Herbert**, “Structure and spectroscopy of the hydrated electron”
10:00-10:15 *Discussion*
10:15-10:30 Break
10:30 -11:00 **Ondrej Marsalek**, “Unraveling the complex nature of the hydrated electron”
11:00-11:15 *Discussion*
11:15 -11:45 **Benjamin Schwartz**, “What can theory and experiment tell us about the structure of the hydrated electron?”
11:45-12:00 *Discussion*
Thursday Evening (6:00 – dark)
Picnic