



**Division of Physical Chemistry
American Chemical Society**

Electrolytes at Charged and Metallic Surfaces

**Julianne M. Gibbs
Richard C. Remsing**
Organizers

San Diego Convention Center
see schedule for room locations

24-27 March 2025

PHYS Programs also available online:



MONDAY AFTERNOON

Structure

J. Gibbs, R. C. Remsing, *Presiding* | **Hall F, Room 3**

2:00 PM. Opening Remarks.

2:10 PM. Insight into the electrical double layer at oxide-electrolyte interfaces from machine learning simulations. C. Zhang, R. Car, **A. Selloni**

2:50 PM. Lithium-ion transport in hybrid electrolytes composed of inorganic electrolyte particles and high-concentration liquid electrolytes. **D. Yu**, B.D. McCloskey

3:10 PM. Interpreting differential capacitance profiles of ionic liquid and concentrated aqueous electrolyte interfaces with a generalized Helmholtz model. **J.G. McDaniel**

3:50 PM. Break.

4:20 PM. Can we exploit hydrophobicity to regulate the chemistry at electrified metal-water interfaces? **S. Pezzotti**

5:00 PM. Capacitive performance of solid-state superionic conductors using constant potential molecular dynamics simulations. **H. Dhatarwal**, K. Wielowski, R.C. Remsing

5:20 PM. Elucidating the potential-dependent structure of hybrid electrolyte/metal electrode interfaces during hydrogen evolution. **M. Waegele**

TUESDAY MORNING

Interfacial Probes

R. Speelman, *Presiding* | **Hall F, Room 3**

8:00 AM. Frustrated hydrogen bonds, sluggish ion dynamics, electric fields, and hydration at metal-electrolyte interfaces. A. Maitra, A.K. Pennathur, C. Tseng, T. Majumder, A. Sarkar, **J. Dawlaty**

8:40 AM. Polar adsorbates' effect on electrostatic potentials in the double layer. **L. Nowack**

9:00 AM. Time-resolved SFG vibrational spectroscopy reveals surprises in the Stark tuning slope for CO on copper. **J. Rebstock**, A. Rao, A. Samanta, A.R. Asthagiri, L. Baker

9:20 AM. Break.

9:50 AM. Water and electrolyte structure and dynamics on the gold electrode surface with adsorbed 4-mercaptobenzonitrile from molecular dynamics simulations. **A.A. Kananenka**

10:10 AM. Characterizing hydrogen bonding in DMSO/water cosolvent mixtures at the gold electrode interface. **C. Baiz**

10:30 AM. Vibrational sum frequency spectroscopy of centrosymmetric molecular ions at aqueous-oxide interfaces. **E. Borguet**

TUESDAY AFTERNOON

Solvation, Fields, and Assembly

H. S. Dhattarwal, *Presiding* | **Hall F, Room 3**

2:00 PM. Electrosolvation force: an emerging paradigm in fluid-phase interactions. **M. Krishnan**

2:40 PM. From Ion ordering to Microphase separation: how charge frustration organizes ions at surfaces. **M. Zhang**, B.A. Helfrecht, Y. Zhang, S. Tan, V. Prabhakaran, Y. Min, C. Mundy, B. Legg, J.J. De Yoreo

3:00 PM. Exploring the connection between electrostatic potential profiles and electric fields within the electric double-layer. **A. Willard**

3:40 PM. Break.

4:10 PM. Molecular strategies to tune the electrode-electrolyte interface for energy storage and conversion. **V. Thoi**

4:50 PM. Stable surfactant monolayers at the electrochemical interfacial double layer across a wide potential range. **C. Wang**, C. Yu, W. Xiong

5:10 PM. Collective effects of electrolytes in bulk and at interfaces. **C. Mundy**

WEDNESDAY MORNING

Evolution of the Interface

J. Rebstock, *Presiding* | **Room 32B**

8:00 AM. Evolution of electrode interfaces during electrochemistry.

Z. Fakhraai, M. Tanwar, H. Fang, C. Cappuccino, T. Taylor, T. Robinson, D.E. Polyansky, M.R. Lockett

8:40 AM. Microscopic origin of twist-dependent electron transfer rate in bilayer graphene. **D. Limmer**

9:20 AM. Bridging electrochemistry and nonlinear optics: Studying the oxygen evolution reaction using second harmonic generation.

R. Speelman, F. Geiger

9:40 AM. Break.

9:50 AM. Chemistry when physics is expected to: Direct spectroscopic probe of electrochemical pseudocapacitive pH jump at a graphene electrode. **M. Bonn**, Y. Nagata, Y. Wang

10:10 AM. Anomalous proton transport in edge-functionalized hexagonal boron nitride membranes. **A. Das**

10:30 AM. Evolution of the electric double layer of silica in aqueous solution. A. Marchioro, **S. Roke**

10:50 AM. Counting ions and net-aligned water molecules at interfaces under electrochemical control using phase-resolved nonlinear optics. **F. Geiger**

WEDNESDAY AFTERNOON

Modeling Electrolyte Interfaces

L. Nowack, *Presiding* | **Room 32B**

2:00 PM. Are extended defects one of the major causes of electronic conductivity in solid electrolytes? **P. Canepa**

2:40 PM. Deciphering the relationship between electric double layer structure and capacitance. **H. Kim**, S. Shin, M.M. Kim

3:00 PM. Atomistic modeling of reaction fields at electrode/aqueous electrolyte interfaces. **J. Nauman**, A. Willard

3:20 PM. Break.

3:50 PM. PW-SMD: Plane-wave solvation model based on electron density for interfacial chemistry. Y. Wang, C. Teng, E. Begin, **J. Bao**

4:10 PM. Regional quantum embedding for adsorbates at metal surfaces. **A. Farahvash**

4:30 PM. Simulations of electrochemical systems with flexible electrode models. **Z. Waysenson**, A. France-Lanord, A. Serva, M. Salanne, A. Saitta

4:50 PM. Accurate descriptions of liquid-solid interfaces with classical density functional theory. **S.J. Cox**, A. Bui

THURSDAY MORNING

Interfacial Reactivity

Z. Waysenson, *Presiding* | **Room 32B**

8:00 AM. Identifying the water structure in the electrical double layer at charged oxide-electrolyte interfaces. **J.M. Gibbs**

8:40 AM. Electrical double layer and lubrication in water-in-salt electrolytes. **J. Frechette**

9:20 AM. Lattice vibrations at interfaces probed by sum-frequency spectroscopy. **W. Liu**

10:00 AM. Break.

10:30 AM. Modulating water activity within aprotic electrolytes for selective CO₂ and CO electrocatalysis. **C. Amanchukwu**

11:10 AM. How potential dependent Multiscale structure creates high hydrogen evolution reaction activity on Pt(111). **R. Campen**, Y. Tong, Z. Huang, G. Zwaschka

11:50 AM. Closing Remarks.

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