Division of Physical Chemistry
American Chemical Society

Molecular Level Understanding of Structure and Dynamics at Electrochemical Interfaces

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Walter E. Washington Convention Center
Room 152A

18-20 August 2025

PHYS Programs also available online:

MONDAY MORNING
Interfacial Spectroscopy & Microscopy

J. Dawlaty, T. Lian, *Presiding*

8:00 AM. Imaging electrochemistry with single molecule resolution using scanning tunneling microscopy. **E. Borguet**

8:30 AM. Probing the spatial distribution of an organic cation in the electrochemical double layer. **M. Waegele**

9:00 AM. Time-resolved SFG vibrational spectroscopy of CO on copper electrodes. **L. Baker**, J. Rebstock, A. Samanta, A. Rao, A.R. Asthagiri

9:30 AM. Quantifying Stern layer water alignment before and during the oxygen evolution reaction. **F. Geiger**

10:00 AM. Intermission.

10:10 AM. Ultrafast aqueous electric double-layer dynamics. **M. Bonn**, A. Greco, S. Imoto, J. Hunger, E. Backus, Y. Nagata

10:40 AM. Sum frequency generation microscopy of electrochemical interfaces. **S. Baldelli**

11:10 AM. Solvation dynamics at the surface of an electrode using voltage-gated 2D IR spectroscopy. **M.T. Zanni**

11:35 AM. Probing water structure at charged graphene interfaces. R. Rashmi, **F. Paesani**

MONDAY AFTERNOON

Interfacial Spectroscopy & Microscopy

J. Dawlaty, Y. Yang, *Presiding*

2:00 PM. Calcite-assisted localization and kinetics (CLocK) microscopy for probing nanoparticle interfaces in electrochemical environments. **K.A. Willets**

2:30 PM. Band gap renormalization effects on electrochemical currents at 2D semiconductor/ electrolyte interfaces. **J. Sambur**, R. Almaraz, A. Tews, T. Sayer, J. Toole, A. Montoya Castillo

3:00 PM. Electroanalytical techniques to better understand nanoscale phenomena in printable semiconducting materials for energy conversion and storage and biosensing. **E.L. Ratcliff**

3:30 PM. Molecular level understanding of ionomer interfaces using Ambient Pressure XPS under in-situ and operando conditions. **P. Aydogan Gokturk**

4:00 PM. Intermission.

4:20 PM. Probing the local electrochemistry of hydrogen evolution on platinum using scanning electrochemical cell microscopy. **H. Ren**

4:50 PM. Operando EC-STEM probing nanoscale dynamics under CO_2 reduction. **Y. Yang**

5:20 PM. Impedance and noise as non-invasive and non-perturbing tools for investigating buried interfaces of electrochemical devices. **B. Ulgut**

TUESDAY MORNING
Advanced Theoretical & Simulation Methods
J. G. McDaniel, A. Willard, *Presiding*

8:00 AM. Electrostatic and solvophobic modulated reaction kinetics for anodic transformation of benzyl alcohols to benzaldehydes. J. Hymel, **J.G. McDaniel**

8:30 AM. Electrified interfaces between water and semiconductors from first principles. **G.A. Galli**

9:00 AM. Machine learning ab initio forces at the solid-liquid interface under applied potential. **M. Galib**

9:30 AM. Timescales at electrochemical interfaces: a perspective from bulk dielectric spectroscopy. **K. Schwarz**

10:00 AM. Intermission.

10:10 AM. Reaction dynamics of solvent decomposition in Li-ion batteries with machine learning potentials. **S. Kundu**, T.C. Berkelbach

10:30 AM. AI acceleration of AIMD simulation of electrochemical interfaces. J. Zhu, F. Tang, **J. Cheng**

11:00 AM. Liquid structure at solid surfaces with arbitrary morphology: A classical superposition model. **Y. Zhang**

11:30 AM. Probing charge transfer and reactions at electrified water-solid interfaces using ab initio thermopotentiostat. **E.M. Lee**

WEDNESDAY MORNING
Interfacial Structure & Dynamics

M. Jackson, A. Willard, *Presiding*

8:00 AM. Electric fields and proton-coupled electron transfer at electrochemical interfaces.
S. Hammes-Schiffer

8:30 AM. Ion creation and destruction in electrochemical reactions. **A. Peterson**

9:00 AM. Interfacial quantum electric fields.
S. Kathmann

9:30 AM. Brønsted slopes and symmetry factors of linear free energy relations for thermal and electrochemical reactions at interfaces. **J.M. Mayer**, J.L. Lee, N. Gibson, R. Agarwal, C. Quist, A. Saha, M. Taylor

10:00 AM. Intermission.

10:10 AM. Mechanism of proton-insertion coupled electron transfer with metal oxides. **V. Augustyn**

10:40 AM. Electrochemical, spectroscopic, and acoustic techniques for the in situ study of 4–mercaptobenzonitrile self-assembled monolayers. **E.M. Nichols**

11:10 AM. Characterizing disorder of and at catalytic electrode materials with in-situ vibrational spectroscopy. **A. Wuttig**

11:40 AM. Electrochemistry @ scale through operando characterization. **Q. Li**, H.D. Abruna

WEDNESDAY AFTERNOON

Interfacial Reactions

A. Hall, Y. Surendranath, *Presiding*

2:00 PM. Role of hydrogen bonding at an electrified metal surface in limited water electrolytes. **V. Thoi**

2:30 PM. Electro-inductive effect. **M. Baik**

3:00 PM. Real-time control of interfacial dynamics enables electrocatalytic C-H and C-C bond transformation and fuel formation. **M. Schreier**

3:30 PM. Probing field effects at photo(electro)catalyst/ solution interfaces. Z. Wang, T. Bo, Q. Huang, C. Ni, F. Fan, **M.V. Mirkin**

4:00 PM. Intermission.

4:20 PM. Insights into the role of the electrode in controlling the selective oxidation of benzyl alcohols. **M. Neurock**, K. Liu, E. Feng, Q. Jing, K.D. Moeller

4:50 PM. Building an all-organic molecular graphite from the ground up. J. Lee, N. Lara, N. Druffner, **M. Jackson**

5:20 PM. Promoting CO_2 reduction by tuning the activity of H_2O. **A. Hall**

The organizers acknowledge the following sponsor for their generous support:

The Journal of Chemical Physics