

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Monday PM

McCormick Place Convention Center W186a

L. Wang, *Organizer, Presiding*

2:00 PM. Evolution of electrode interfaces during electrochemistry. **Z. Fakhraai**, M. Tanwar, H. Fang

2:25 PM. Measuring the capacitive response of ionic liquids and metallic electrodes. **S.K. Shaw**

2:40 PM. Ion pairing in confined aqueous electrolytes. **S. Dasgupta**

2:55 PM. 10 min break.

3:05 PM. Solvent-exchange kinetics govern ion pairing in Na-ion electrolytes: Insights from OMol-trained machine learning potentials. **N. Kumar**, J. Lai, E. Crumlin, S. Blau

3:20 PM. Underscreening and electrostatics of electrolytes in bulk and at interfaces. **C. Mundy**, M. Dinpajoo

3:45 PM. 20 min break.

4:05 PM. Identifying the electrical double layer structure at charged oxide/electrolyte interfaces. **J. Gibbs**

4:30 PM. Interrogating the speciation of aqueous ZnCl_2 through experimental and theoretical spectroscopy. **L. Gibson**, C. Lin, J. Chen, M.D. Baer, J. Fulton, C. Mundy,

P.S. Cremer, M. Dinpajoo

4:45 PM. Resolving the structure of high concentration lithium ion electrolytes using localized (midIR) and delocalized (THz) vibrational modes. **D.G. Kuroda**, M. González-Jiménez, K. Wynne

5:10 PM. 10 min break.

5:20 PM. Ion-specific transport phenomena in polymer electrolytes: Vibrational spectroscopic and rate theoretical insights. **S. Roy**, U.I. Premadasa, J. Foster, B. Doughty

5:35 PM. Operando measurements of the formation of the solid electrolyte interphase in operando with sum-frequency generation. **J.D. Cyran**

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Tuesday AM

McCormick Place Convention Center W195

S. Roy, *Organizer, Presiding*

8:00 AM. Solvation at liquid/liquid interfaces. **B. Doughty**, P. Sun, J. Carrillo, U.I. Premadasa, R.L. Sacci, S. Roy

8:25 AM. Where is the salt? Sensing the ionic environment of the air-water interface at the molecular-level using a vibrational probe. S. Parsons, K. Judd, D. Eremin, V.V. Fokin, **J. Dawlaty**

8:40 AM. 10 min break.

8:50 AM. Remotely controlled interfacial pH gradients using photoacid surfactants. **U.I. Premadasa**, Y. Ma, S. Decatur, Y. Liao, V. Bryantsev, R.L. Sacci, B. Doughty

9:15 AM. Effect of trace water on ion transport through immiscible liquid-liquid interfaces: Microscopic pictures from free energy analysis. **A. Morita**

9:40 AM. 20 min break.

10:00 AM. Aqueous interfacial hydration environments of ions and surfactants by phase - second harmonic, sum frequency, infrared reflection, and Raman spectroscopies.

H.C. Allen, N. Adhikari, B. Biswas, G. Nieto, T. Bowling-Charles, J. Badjic

10:25 AM. Nucleation and growth in electrolyte systems. **S. Sarupria**, P. Minh, T. Tan

10:40 AM. Small is beautiful: Ultrananoscale, engineered active site directing charge flow in complex systems. **M.J. Shultz**, Z. Lin, R. Talukder

11:05 AM. 10 min break.

11:15 AM. Quantifying interfacial ionic properties in ionomer-coated electrocatalysts. **J. Urbine**, S. Ardo

11:30 AM. Ionic double layer at the air-water interface. I. Mezghani, A. Gonzalez Sanz, M. de la Puente, **D. Laage**

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Wednesday AM

McCormick Place Convention Center W185a

Z. Fakhraai, *Presiding*

8:00 AM. Non-thermal aging of supercooled liquids in optical cavities. **N. Hoffmann**

8:25 AM. Probing the bending mode of water with tip-enhanced vibrational spectroscopy. **E.A. Muller**, I. Kats-Rodgers

8:40 AM. Quantum proton delocalization in organic acid-1-methylimidazole binary mixtures. R. Zhang, A. Gurung, D.G. Kuroda, **L. Wang**

8:55 AM. 10 min break.

9:05 AM. Correlating solvation shell dynamics to bulk scale ion motion in polymeric membrane. **R. Ball**, J.M. Anna, C.O. Osuji, A. Patel, L. Zhang, C. Johnson, R. Hopkins

9:20 AM. Two molecular pathways for ion-driven “structure making / breaking” in water revealed by Correlated Vibrational Spectroscopy. **P. Singh**, V. Vorobev, M. Flor, S. Roke

9:45 AM. 20 min break.

10:05 AM. Orbmol-v2: Learnable and efficient electrostatics for universal neural network potentials. **T. Duignan**

10:30 AM. From bulk speciation to interfacial desolvation kinetics: a molecular framework for battery electrolyte design. **N. Rampal**, S.E. Weitzner, C. Orme, L. Wan

10:45 AM. Vibrationally resolved electronic spectra from Hagedorn wavepacket dynamics. **J. Vanicek**

11:10 AM. 10 min break.

11:20 AM. Visualizing solvation dynamics in ionic liquids with *ab initio* accuracy for battery science. **A.J. Dominic**, A. Montoya Castillo

11:35 AM. Molecular-level interpretation of the voltage- and electrolyte-dependent dynamics of 4-MBN monolayer on the gold electrode and the nitrile stretch frequency shifts. **A.A. Kananenka**

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Wednesday PM

McCormick Place Convention Center W185a

Y. Jiang, *Presiding*

2:00 PM. First hydration shell integrity: Key to protein stability. Z. Wang, M. Tremblay, N. Hatzis-Schoch, T. Zhu, S. Hammes-Schiffer, **E.C. Yan**

2:25 PM. Docking-based simulation of cell-size systems with flexible protein structures. **A. Singh**, K. Yunas, A.M. Tytarenko, M.M. Copeland, P. Kundrotas, P.O. Kasyanov, E.A. Feinberg, I.A. Vakser

2:40 PM. Tracking hidden dynamics: From weakly-bound water to protein surface motifs and drug-crystal rigidity by ultrafast 2D IR spectroscopy. **J. Wang**

2:55 PM. 10 min break.

3:05 PM. Mapping Heterotypic Amyloid Interactions With Infrared Spectroscopic Imaging. **A. Ghosh**

3:20 PM. Quantifying protein secondary structure with 2D IR spectroscopy and transition dipole strength analysis. **L.E. Buchanan**

3:45 PM. 20 min break.

4:05 PM. Molecular mechanism of large-scale conformational transition in Arp2/3 complex. **S. Sridharan Iyer**, J. Wu, T. Pollard, G.A. Voth

4:30 PM. Site-specific and Mode-specific Photodissociation of OH bonds in a Pentapeptide by laser-driven Tunneling through a Conical Intersection. K. Au, I. Ofori, K. Woo, D.M. Leitner, M.A. Kubasik, L.V. Slipchenko, **T.S. Zwier**

4:45 PM. Tackling the many ferredoxins problem in *Chlamydomonas reinhardtii* with molecular simulations and AI Structural Biology. C. Hofstrand, J. Nguyen, D. Sarkar, C. Fischer, S. Schmollinger, D. Strenkert, **J.V. Vermaas**

5:00 PM. 10 min break.

5:10 PM. Coupled conformational dynamics and multisite proton-coupled electron transfer in ribonucleotide reductase. **J. Deng**, S. Hammes-Schiffer

5:25 PM. Membrane potential modulation of bacterial small-molecule transport. **T.R. Calhoun**, E. Campbell

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Thursday AM

McCormick Place Convention Center W184bc

A. Ghosh, *Organizer, Presiding*

8:00 AM. How molecular structure governs intersystem crossing in firefly luciferin and beyond. **R. Tempelaar**, A. Garzon-Ramirez

8:25 AM. Dark state-mediated photobleaching in mCherry-based red fluorescent proteins. **P. Manna**, S. Mukherjee, M. Hix, A. Walker, R. Jimenez

8:40 AM. Impact of A-Motif formation on Adenine excited-state decay: A comparison with single-stranded DNA. **W. Kwok**, A. Law, J. Chow, Q. Xiong, C. Ma

8:55 AM. 10 min break.

9:05 AM. Time-resolved 2D IR spectroscopy reveals $n \rightarrow \sigma^*$ interaction dynamics in the SET7/9 methyltransferase active site. **Z. Nikolaidi**, H.E. Rice, K.E. Helme, R. Krishnan, R. Knierim, T.D. Hill, S. Basnet, J. Fontaine, D. Woodfill, R.C. Trievel, **S.D. Moran**

9:20 AM. Trapping single biomolecular nanoparticles in solution. **W. Carpenter**

9:45 AM. Break.

10:30 AM. Determining redox thermodynamics and kinetics in coacervates. **L. Sepunaru**

10:45 AM. Unveiling the dynamic nature of phase-separating protein-peptide complexes via AI and MD. **S. Kim**

11:00 AM. 10 min break.

11:10 AM. Revisiting diffusion-controlled association kinetics: From single-molecule adsorption to bulk reaction models. S. Pandey, **J. Chen**

11:25 AM. Integrating correlated motion and energy flow network analyses to elucidate long-range dynamic communication in soybean lipoxygenase. **Y. Jiang**, J. Cordova, J. Yuan, J. Klinman

11:40 AM. Interpretable deep learning and causal inference decipher mechanisms of RNA-guided transposition. **G. Palermo**, C. Pindi, M. Ahsan, S. Sinha

Dynamic Processes in Electrolytes and Biomolecular Systems

Organizers: Santanu Roy, Richard Remsing, Lu Wang, and Ayanjeet Ghosh

August 24-27, 2026

Special Thanks to our Sponsors



Contact: Eric Kennehan Email: erkennehan@maginsts.com

www.magnitudeinstruments.com



PhaseTech Spectroscopy, Inc.

Contact: Chris Middleton, Email: chris.middleton@phasetechspectroscopy.com



Contact: Art Camire Email: art.camire@mks.com

<http://www.spectra-physics.com>

<http://www.mks.com>