

2021 Molecular Electrochemistry MURI Review

All oral presentations by ZOOM: Meeting ID: 969 9508 0679 , Password MURIreview
<https://emory.zoom.us/j/96995080679?pwd=M2pNZ0hYK3JTYUwxeHBrZWREUT09>

Poster sessions: Spatial Chat (<https://spatial.chat/s/MURI-2021>)

8/9/2021	Speaker	Title
9:00 – 9:10 am	Mike Berman	Opening remarks
9:10 – 9:20 am	Tim Lian	MURI overview
9:20 – 9:55 am	Yogi Surendranath	Understanding the pH-dependent kinetics of H ₂ evolution catalysis
9:55 – 10:30 am	Sharon Hammes-Schiffer	Electric Fields and Proton-Coupled Electron Transfer at Electrochemical Interfaces
10:30 – 10:45	Coffee Break	
10:45 – 11:20 am	Jahan Dawlaty	Tracking Mechanistic Details of the Volmer Reaction using a Stark Probe
11:20 – 11:55 am	Jim Mayer	Protons, electrons and HER on gold — nanoparticles and electrodes
11:55 – 12:30 pm	Patrick Unwin	Correlative Electrochemical Multi-Microscopy: Understanding Electrochemical Interfaces from Local to Global
12:30 – 1:30 pm	Lunch Break	
1:30 – 2:00 pm	Poster talks	1 minute /1 slide per poster (Zoom meeting)
2:00 – 3:30 pm	Poster session 1	Posters 1-5 (Spatial Chat Room 1), Posters 6-10 (Room 2)
3:30 – 5:00 pm	Poster session 2	Posters 11-15 (Room 3), Posters 16-19 (Room 4)
8/10		Zoom
9:00 – 9:35 am	Tito Abruna	Electrons, Ions and Photons; Mechanistic Studies of Electrochemical Transformations
9:35 – 10:10 am	Adam Willard	Simulating nanoscale potential fluctuations within the electric double layer
10:10 – 10:45 am	Tim Lian	Operando probe of ion adsorption on electrodes: from battery to CO ₂ reduction
10:45 – 11:00 am	Coffee Break	
11:00 – 11:35 am	Joe Subotnik	Methods for Cyclic Voltammetry and Progress Towards Ab Initio Nonadiabatic Electrochemical Studies
11:35 – 12:10 am	Jesse McDaniel	Aqueous vs Ionic Liquid Double Layers: Incorporating Electric Fields in Computational Electrochemistry
12:10 - 12:30 am	Open discussion	
12:30 pm	End of meeting	
1:30 – 3:30 pm	PI only	Cornerstone Project Discussion (Zoom meeting)
1:30 – 5:00 pm	student/postdoc only	Poster session and team building (Spatial Chat)

- All talks are 25 minutes + 10-minute discussion

For updated meeting schedule, please check:

<https://scholarblogs.emory.edu/echemmuri/muri-annual-review-meeting/>

2021 MURI Meeting Poster Sessions in SpatialChat

Full Name	Status	Institutional Affiliation:	Poster Title
POSTER ROOM 1			
Rishi Agarwal	Grad Student	Yale University	DEMS Study of Product Isotope Effects in the Hydrogen Evolution Reaction
Dhritiman Bhattacharyya	Postdoc	Emory University	Mapping the electric field strength inside an electric double layer using a molecular ruler.
Alec Coffman	Grad Student	University of Pennsylvania	A grid-free approach for simulating sweep and cyclic voltammetry
Phillips Hutchison	Grad Student	Yale University	Modeling Proton-Coupled Electron Transfer Thermodynamics and Kinetics Using Constant Potential DFT
Onyu Jung and Bryan Tang	Grad Student and Undergrad	MIT	Kinetics of Hydrogen Evolution on Pt, Au, and Pd
POSTER ROOM 2			
William Lake	Grad Student	Yale University	Theoretical Studies of Interfacial Electric Fields using Vibrational Probes and Redox-Active Molecules
Chaoyu Li	Postdoc	Emory University	Revealing the electric double layer structure in highly concentrated aqueous electrolytes
Aditya Limaye	Grad Student	MIT	Characterizing Electrochemical Systems By Volterra Kernel Analysis of Response to Small-Amplitude Oscillatory Voltage Inputs
Xinyao Lu	Grad Student	Cornell University	kinetic isotope effects on hydrogen electro-adsorption on Pt(111) in alkaline media
Anwasha Maitra	Grad Student	University of Southern California	Electric Fields at Metal-Surfactant Interfaces: A Combined Vibrational Spectroscopy and Capacitance Study
POSTER ROOM 3			
Sevan Menachekanian	Grad Student	University of Southern California	How does a Classic Lewis Adduct Behave at an Interface?
Jinhui Meng	Grad Student	Emory University	Integrated in situ Molecular Spectroscopic and Computational Study of Electrochemical Interfaces
Linsey Nowack	Grad Student	MIT	Modeling CO ₂ reduction adsorbates on a Cu electrode
Tian Qiu	Postdoc	University of Pennsylvania	Towards nonadiabatic electronic structure on metal surface
Sohini Sarkar	Postdoc	University of Southern California	Mechanistic Insights about Electrochemical Proton-Coupled Electron Transfer Derived from a Vibrational Probe
POSTER ROOM 4			
Dylan Suvlu	Postdoc	MIT	Potential fluctuations around a polarizable model of gold nanoclusters
Matthew Voegtle	Grad Student	University of Southern California	Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations Please correct typo
Hongsen Wang	Postdoc	Cornell University	A Combination of DEMS and FTIR Spectroscopy: Application to Study Methanol and Formic Acid Electrooxidation on Pt
Thejas Wesley	Grad Student	MIT	Partial charge transfer governs the electric field dependence of thermochemical catalysis at metal-liquid interfaces