

Attendee Handbook and Program for the 2023 SoCal Electrochemistry Conference for Students

ECS@UCI

April 19, 2023
University of California, Irvine
Irvine, CA, 92697



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1 The Inspiration Behind the 2023 SCECS

Academia has this central, beautiful aspect of community; from it, we learn concepts and techniques and receive guidance and critiques of our research, and with it, we share our discoveries and innovations. In short, to enrich our community is to ultimately enrich ourselves. And yet, there is not enough emphasis on connecting students with other students, even those in their own field. This I find strange. While we are not yet experts (if anyone can claim to be such a thing!), we are professionals in training, we are the next generation. So, why wait 5, 10, 15 years to begin connecting with each other? For most of us, we have the advantage of time and so, if we do it right—bit by bit, year by year—we can eventually become colleagues, collaborators, and, perhaps most of all, friends. We can create a community right here in Southern California, and who knows how far that can take us. And it was out of this philosophy that the 2023 SCECS was born. In addition to the 2 keynotes, 20 talks, and 21 posters, we included many opportunities for you to connect with other attendees, whether it be over a cup of coffee or a glass (or two) of Prosecco. In that spirit, all of us here at ECS@UCI are genuinely excited to host you at UCI and welcome you to the 2023 SCECS.

Warmly,

Christopher Pantayatiwong Liu, President of ECS@UCI

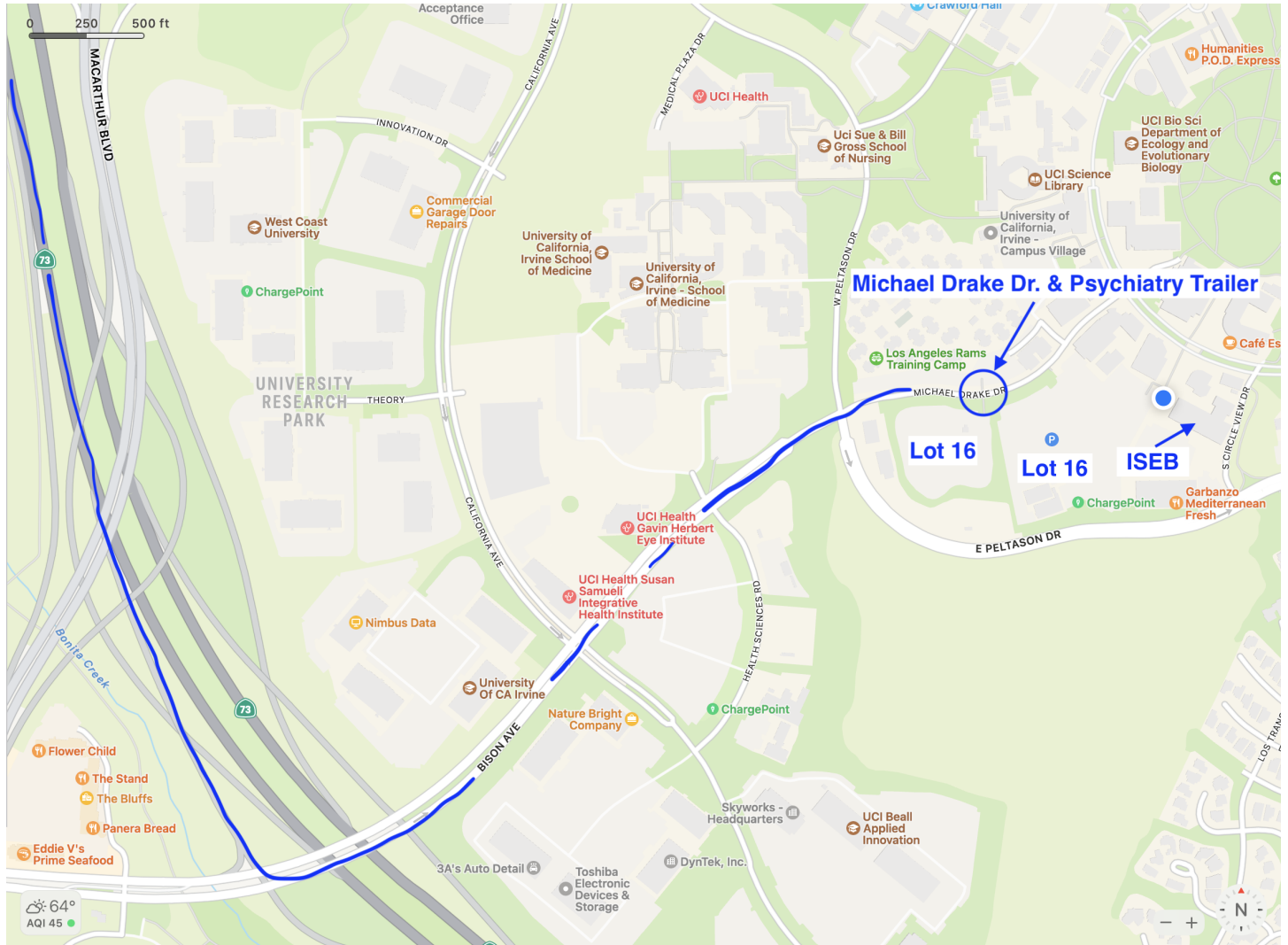
2 Conference Schedule

Time	Event	Location
8:00 - 9:00 a.m.	Check-In	ISEB First Floor Outdoor Plaza
9:00 - 9:50 a.m.	Keynote 1: Adam Z. Weber	ISEB 1010
9:50 - 11:00 a.m.	Poster Session and Coffee Break	ISEB First Floor Lobby
11:00 a.m. - 12:20 p.m.	Session 1A: Electrochemical Sensors Session 1B: Fuel Cells and Electrolyzers	ISEB 1310 ISEB 1200
12:30 - 2:00 p.m.	Lunch	ISEB First Floor Lobby and Outdoor Plaza
2:00 - 2:50 p.m.	Keynote 2: Kimberly A. See	ISEB 1010
3:00 - 4:00 p.m.	Session 2A: Batteries and Energy Storage I Session 2B: Electrocatalysis I	ISEB 1200 ISEB 1010
4:00 - 4:45 p.m.	Coffee Break	ISEB First Floor Lobby
4:45 - 5:45 p.m.	Session 3A: Batteries and Energy Storage II Session 3B: Electrocatalysis II	ISEB 1200 ISEB 1010
6:00 - 7:00 p.m.	Happy Hour	ISEB First Floor Lobby
6:45 p.m. - 8:00 p.m.	Dinner	ISEB First Floor Lobby and Outdoor Plaza

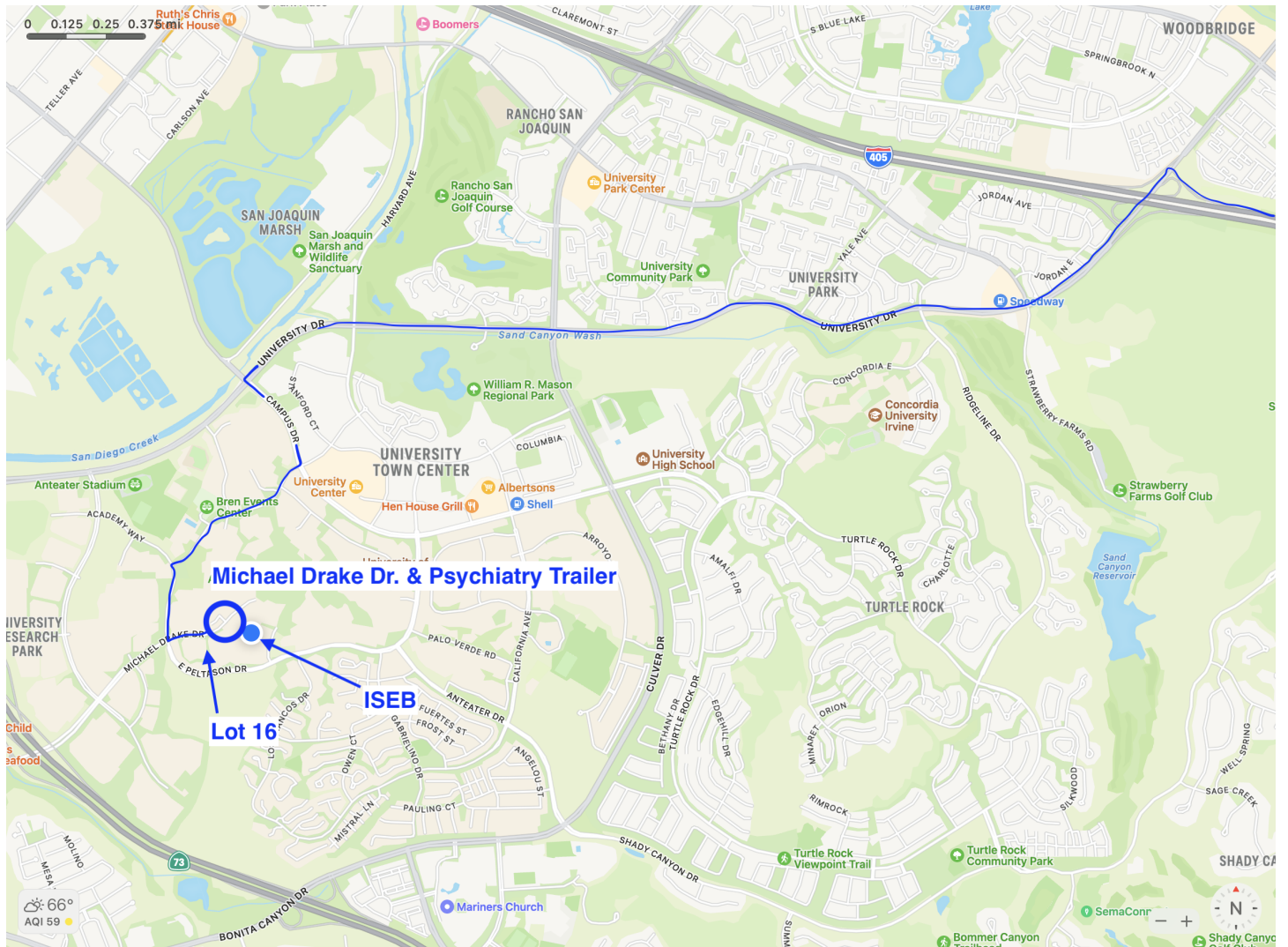
3 Logistics

3.1 Navigating to UCI

The nearest parking to the Interdisciplinary Science and Engineering Building (ISEB) is Lot 16, which itself does not have a defined address. You will want to set your navigation to Michael Drake Dr. & Psychiatry Trailer, which should lead you to a street adjacent to Lot 16. From Lot 16, it is a short walk to ISEB. If you are coming to UCI from the north, you will likely be taking the 73 during your last leg of the drive; be sure to exit the freeway on Bison Ave. as beyond that exit the 73 becomes a toll road. After turning left onto Bison Ave., at the intersection with Peltason Dr. continue straight and to your right will be Lot 16 (Bison Ave. becomes Michael Drake Dr.).

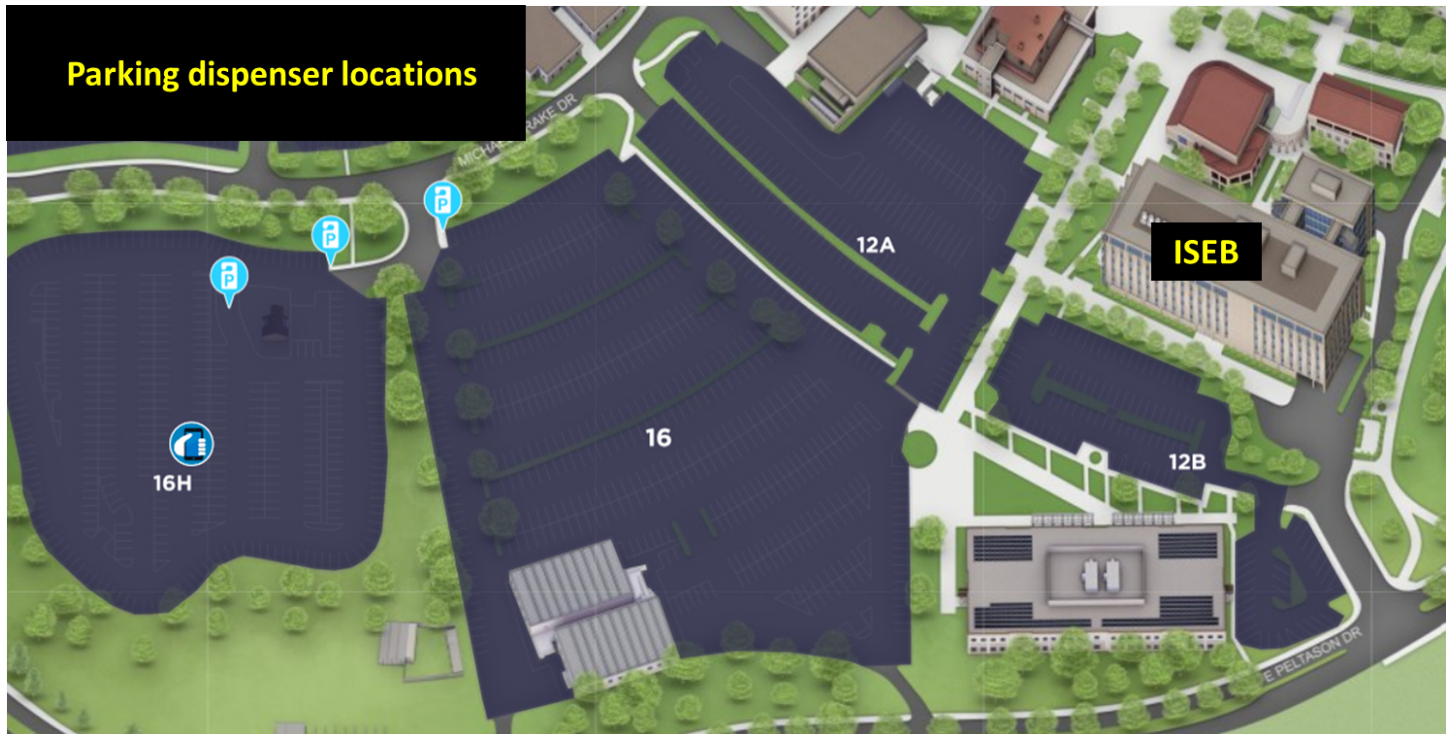


If coming from the south, to avoid paying a toll, do not take the 73 and instead stay on the 5 N to the 405 N and get off on University Dr. Turn left onto Campus Dr., right onto W. Peltason Dr. then make a left at the T-junction. At the next intersection, turn left onto Michael Drake Dr. and Lot 16 will be on your right.



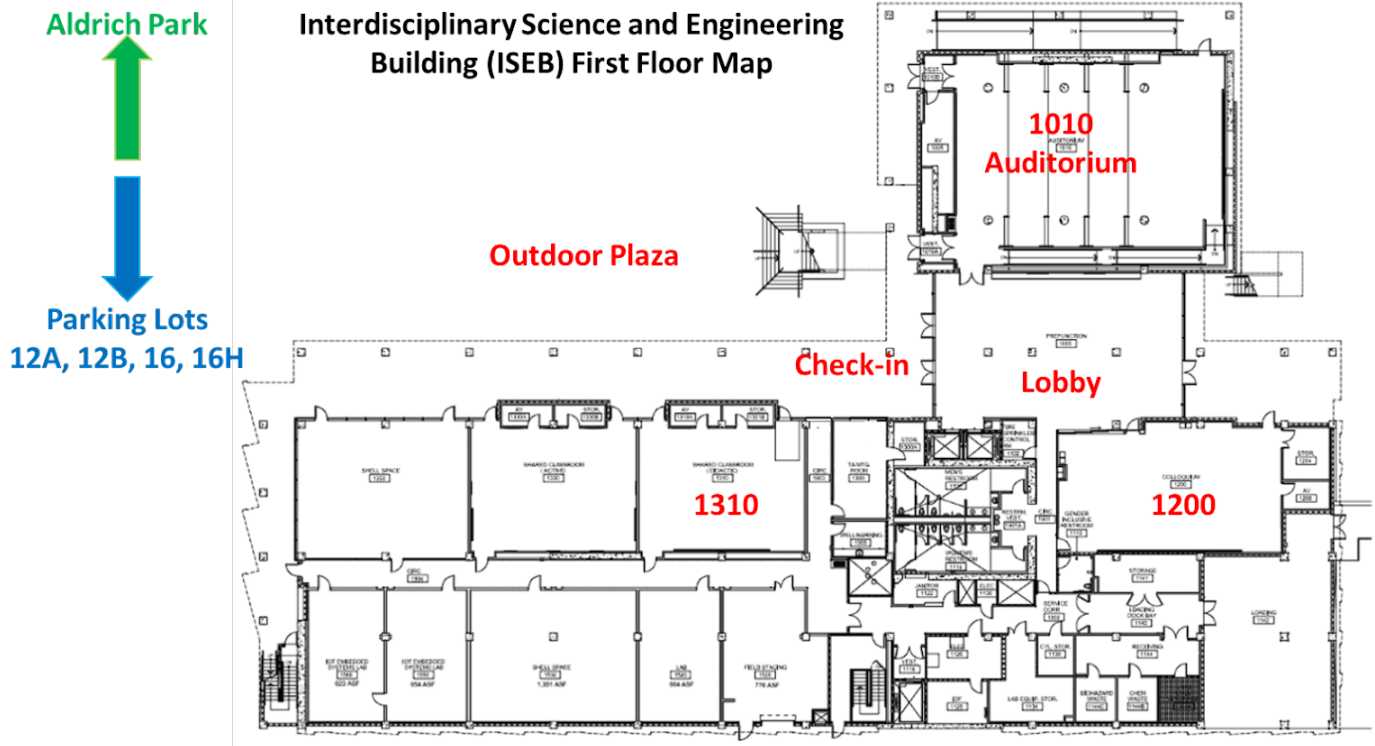
3.2 Parking

“One Day-Reserved” parking passes are \$18; park in stalls that say “AR” (which sometimes have an adjacent red sign), or an unmarked stall. The parking dispenser locations are shown below. More information can be found at <https://parking.uci.edu/permits/visitorpermits.cfm>.



3.3 Conference Building (ISEB) Map

A map of ISEB is shown below.



4 Keynote Speakers

4.1 Keynote 1: Importance of Transport in Electrochemical Energy-Conversion Technologies: Exploring Multi-Species Transport in Ionomers

9:00 - 9:50 a.m.

ISEB 1010

Adam Z. Weber

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Abstract. As electrochemical technologies become increasingly important in our energy paradigm, especially hydrogen, there is a need to examine them holistically. Furthermore, for such technologies to become practical, they need to operate at high current densities to minimize various cell costs. This operating space necessitates the need for efficient transport of reactants and removal of products from the reaction site and in a solid-state architecture that utilizes ion-conducting polymers (ionomers). In this talk, we will explore the various tradeoffs endemic in such gas-diffusion electrode (GDE) architectures for various electrochemical reactions including CO₂ reduction and O₂ and H₂ consumption and evolution. Such tradeoffs are quantified through multiphysics modeling and key diagnostics of the cells including breakdowns of the various limiting phenomena at both the micro and macroscales, where the local conditions and environment around the reaction site impact reactivity in both transient and steady state conditions, enabling metastable states. In addition, we will take a deeper examination into the transport processes within the ionomer itself. While an ideal ionomer in many different technologies is a solid-state single-ion conductor, this is rarely seen in practice where other ions may exist as contaminants, additives, or due to electrolyte solutions. In this talk, we will describe theoretical studies into the nature of multi-ion transport in ionomers. The discussion will start from examining selectivity of ionomers and then transport including conductivity, electro-osmosis, and water diffusion using a self-consistent framework. Focus will be on cation and then anion conducting ionomers, where CO₂ plays a critical role in the latter due to acid/base reactions. Time-permitting, we will then explore different applications including bipolar membranes, where co- and counter-ion crossover present significant obstacles to developing efficient and stable devices. Finally, we will explore different mechanisms on not only ion but also neutral species transport including water using a network methodology to examine specific transport pathways. With such a deep understanding on transport within the ionomer, we will be able to examine the limiting phenomena in different GDE architectures and quantify their intrinsic tradeoffs including complex interplay of hydration, reactant concentration, and both homogeneous and heterogeneous reactions.

Bio. Adam Z. Weber holds B.S. and M.S. degrees from Tufts University, and a Ph.D. at University of California, Berkeley in chemical engineering under the guidance of John Newman. Dr. Weber is a Senior Scientist and Leader of the Energy-Conversion at Lawrence Berkeley National Laboratory, and co-Director of the Million Mile Fuel Cell Truck Consortium. His current research involves understanding and optimizing fuel-cell and electrolyzer performance and lifetime including component and ionomer structure/function studies using advanced modeling and diagnostics, understanding flow batteries for grid-scale energy storage, and analysis of solar-fuel generators and CO₂ reduction. Dr. Weber has coauthored over 200 peer-reviewed articles and 11 book chapters on fuel cells, flow batteries, and related electrochemical devices, developed many widely used models for fuel cells and their components, and has been invited to present his work at various international and national meetings. He is the recipient of a number of awards including a Fulbright scholarship to Australia, a 2012 Presidential Early Career Award for Scientists and Engineers (PECASE), the 2014 Charles W. Tobias Young Investigator Award of the Electrochemical Society, the 2016 Sir William Grove Award from the International Association for Hydrogen Energy, and a 2020R&D100 award for microelectrode development. He is a Fellow of The Electrochemical Society and the International Association of Advanced Materials.

4.2 Keynote 2: One is the Loneliest Number: Multivalent and Multielectron Processes for Next-Generation Batteries

2:00 - 2:50 p.m.

ISEB 1010

Kimberly A. See

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Abstract. Rechargeable Li-ion batteries revolutionized portable energy storage but the limitations imposed by intercalation chemistry, cost associated with precursors of active materials, and critical nature of crucial elements drive the need for new batteries. Our lab aims to develop energy dense chemistries that *obviate* the need for the critical and costly elements like Co and Ni in the cathode and Li as a working ion. The search for these so called “beyond Li-ion” technologies include systems based on alternative charge storage mechanisms that promise high theoretical capacity and energy density. We will discuss how charge storage mechanisms beyond intercalation can be leveraged to yield high energy densities with Fe-based materials. By understanding the fundamental charge storage mechanism in these materials using electrochemical, spectroscopic, and structural characterization tools, we can develop new materials with targeted properties. We will also discuss strategies to go beyond Li working ions looking toward more sustainable ions like Mg^{2+} , Ca^{2+} , and Zn^{2+} . We will take a fundamental look at multivalent ion diffusion in the solid-state: a cornerstone process for the function of multivalent batteries.

Bio. Kimberly See is an Assistant Professor of Chemistry in the Division of Chemistry and Chemical Engineering at Caltech. She was born and raised in Colorado and received her B.S. in Chemistry from the Colorado School of Mines. Kim pursued her Ph.D. in Chemistry at the University of California, Santa Barbara where she worked with Profs. Ram Seshadri and Galen Stucky. Kim was awarded the St. Elmo Brady Future Faculty Postdoctoral Fellowship at the University of Illinois at Urbana-Champaign and worked with Prof. Andrew Gewirth in the Department of Chemistry. Now, her group at Caltech studies new chemistry for next-generation energy storage with a focus on Earth abundant, inexpensive materials. She focuses on the electrochemistry associated with multivalent and multielectron processes. Some of her recent awards include the Beckman Young Investigator Award, VW/BASF Science Award Electrochemistry, Packard Fellowship for Science and Engineering, and the Office of Naval Research Young Investigator Award.

5 Instructions for Presenters

5.1 Poster Presentations

- After check-in, place your poster (no more than 36 in. by 48 in.) at the easel with your assigned poster number. There will be clips and cardboard supports available at every easel. Please make sure your poster number remains visible in the top left corner at all times.
- The posters will remain on the cardboard supports and easels until 4:45 p.m. where they will then be taken by our conference volunteers to the check-in table while still attached to the cardboard supports with the poster number.
- When you're ready to pack up your poster, you can give the check-in table your poster number and they will retrieve the cardboard clipped poster for you.

5.2 Session Talk Presentations

- Please have your talk in PowerPoint or PDF form uploaded onto a USB or in a cloud-shareable format, ideally the former.
- Moderators will be in their respective session rooms 15 minutes before their session begins; please head to your session room to upload your talk with the moderator before your session begins.

6 List of Posters

Time: 9:50 - 11:00 a.m.

Location: ISEB First Floor Lobby

#	Name	Affiliation	Title & Abstract
1	Logan Brennan	University of California, Irvine	FeWO₄ Photoanodes for Photoelectrochemical Oxygen Evolution Reaction
2	Julia Chung	University of California, Santa Barbara	On the Disinfection of Electrochemical-Aptamer Based Sensors Electrochemical aptamer-based (EAB) sensors enable the continuous, real-time detection of drugs and metabolite targets in the body. This platform is simultaneously (1) general, being independent of the chemical or enzymatic reactivity of its target; (2) continuous and lag-free; and (2) selective enough to deploy <i>in-situ</i> in the living body. Accordingly, much interest surrounds EAB sensors as a candidate technology for biomedical research and the diagnosis, treatment, and monitoring of disease. However, utilizing these devices in long-duration animal models, much less in human patients, requires that they be free of any significant pathogen load. Thus motivated, we have characterized the compatibility of EAB sensors with standard sterilization and high-level disinfection techniques. In doing so, we find that, while many cleaning protocols lead to significant sensor degradation, treatment with CIDEX OPA (0.55% ortho-phthalaldehyde) leads to effect disinfection without causing any detectable loss in sensor performance.
3	Andrew Cypcar	University of California, Irvine	Kinetic Inhibition of the Hydrogen Evolution Reaction for Selective CO₂ Reduction Electrocatalysis An emerging technology to mitigate climate change is electrocatalytic conversion of CO ₂ to value-added fuels. While both heterogeneous and homogeneous electrocatalysts can perform this reaction, selectivity for CO ₂ reduction products over the H ₂ evolution reaction (HER) needs to be improved for large-scale implementation. Hydrogen evolution is often more thermodynamically favorable than hydride transfer to CO ₂ , so new kinetic strategies that inhibit protonation of metal hydride intermediates must be developed. Herein, we aimed to develop a homogeneous electrocatalytic system for selective CO ₂ to formate conversion by using steric factors to kinetically inhibit HER. A series of platinum bis(diphosphine) complexes with differing steric hindrance were tested in combination with sterically bulky acids. While these metal hydride complexes have comparable thermodynamic favorability for HER, protonation is inhibited when both a sterically hindered acid and diphosphine ligand are used. This effect could be leveraged for selective electrochemical reductions in the presence of protons.

4	Spencer Delgado	California Institute of Technology	<p>Electrochemical C-C Bond Formation at Rhodium Hydroformylation Catalysts</p> <p>Electrochemical reactions offer the advantage of voltage as a thermodynamic driving force that can be sustainably sourced to produce value-added products. Aldehydes are a valuable synthetic intermediate, being able to be functionalized into a variety of downstream products. An industrially relevant path towards aldehydes is the hydroformylation of olefins at high pressures of syngas (10 bar and above) and temperatures (80 °C and above). This work investigates the mechanism of electrochemical hydroformylation (electro-HFN), the faradaic counterpart to hydroformylation (thermo-HFN). Known heterogeneous Rh-based catalysts for thermo-HFN are imported onto an electrode surface, resulting in a catalytic cycle utilizing electrons and protons directly, in contrast to hydrogen gas as a traditional reductive source. Kinetic data is consistent with distinct electron transfer and proton transfer steps in the catalytic cycle, while <i>in-situ</i> x-ray absorption spectroscopy shows rhodium active sites do not undergo a change in oxidation state under reaction conditions. Through investigation of substrate scope, understanding of the surface interactions at active sites and understanding of the mechanism at key faradaic steps is progressed. Electro-HFN operates at mild conditions compared to thermo-HFN but must continue to be optimized through rational design.</p>
5	Joseph Gott and Miguel Orozco	University of California, Santa Barbara	<p>The Heterogeneity of Turn-Over Number in Electrocatalysis</p> <p>Chemical catalysts dominate the multi-billion global revenue of the chemical industry because they accelerate the time it takes a reaction to reach equilibrium without altering the equilibrium constant. From a techno-economical point of view, some considerations are critical during a catalyst design: cost, activity, and durability. Turnover number (TON) is one way to quantify catalyst durability, representing the maximum yield of products attainable from a catalytic center. Currently, without any exception, the TON is given as a fixed number describing the total amount of substrate converted until the catalysts fully degrade. We share here some preliminary results showing that electrocatalyst degradation is heterogeneous, where some are more stable than others. To achieve this goal, we use single-entity electrochemistry to study electrocatalytic deactivation processes when single nanoparticles impact the electrode. By measuring the current decay response of a single platinum nanoparticle during the hydrogen evolution reaction, we show that the TON is inherently heterogeneous and depends on the applied potential and size of the nanoparticles. Once this technique is fully developed, we will apply this electroanalytical technique to other electrocatalysts. We hope this redefinition of turnover numbers will assist in the bottom-up approach of materials development toward large-scale industrial electrocatalysis.</p>

6	Sierra Gross	University of California, Irvine	<p>Morphological Design of Silicon Anodes for Lithium-Ion Batteries Alloying type anodes for lithium-ion batteries, such as silicon, are desirable due to their high theoretical capacity; however large volume variations (~300 vol% for Si) during cycling can lead to mechanical degradation and loss of active material, resulting in an overall decline in electrochemical performance. Efforts to address these issues include the use of nanostructures and composites, which can require complex synthesis routes and decrease active material loading. An alternative route is to utilize thin coatings of active material on bicontinuous porous architectures. This allows for a balance of power and energy density, while simultaneously maintaining mechanical integrity. This project uses finite element analysis to study the mechanics of Si layers coated on spinodal, inverse opal, gyroid, and Schwartz primitive nickel backbones during expansion in order to explore the importance of surface curvature and morphology. This presentation highlights the promise of spinodal structures for alleviating expansion-induced mechanical degradation while also being amenable to scalable synthesis routes.</p>
7	Emma Hopkins	University of California, San Diego	<p>Electroless Plating of High-Aspect-Ratio Substrates for TF-SOFCs A fully conductive, nanoporous substrate for thin-film solid oxide fuel cells (TF-SOFCs) is demonstrated <i>via</i> the use of electroless Ni plating. TF-SOFCs achieve high power density at lower temperatures than conventional SOFCs with the use of nanoscale sputtered films that reduce the ohmic resistance of each layer in the cell stack. Nanoporous Al₂O₃ is commonly used as a substrate for TF-SOFCs due to its high temperature stability and aligned, nano-sized pores. This allows for both conformal sputtering on the surface and efficient fuel delivery to the anode. Problematically, Al₂O₃ is insulative, inhibiting effective current collection on devices larger than 1 cm². A conductive nanoporous substrate would simplify stack design by allowing efficient current collection across the entire substrate. This also decreases the likelihood of cell failure <i>via</i> warping, by reducing the difference in the coefficients of thermal expansion (CTEs) between the anode and substrate. This work outlines the use of an electroless plating method on a high-aspect ratio nanoporous Al₂O₃ substrate, wherein full conductivity is achieved <i>via</i> the deposition of a continuous Ni-P layer.</p>

8	Stefan Ingvarsson	University of California, Santa Barbara	<p>Electrochemistry of Xylem and its Possible Applications in Calcium Transport</p> <p>Xylem fibers are vital components of a plant's water and ion transport system, which are essential for maintaining plant growth and development. However, little is known about their ex vivo ionic conductivity properties. In this study, we used Cyclic Voltammetry (CV) and Mass Spectrometry (MS) to characterize the electrochemical activity of isolated xylem fibers, which were found to be redox active in solution. We hypothesize that adding a supporting electrolyte can enhance the ionic conductivity in xylem fibers, surpassing the biological ionic conductivity reported in the literature. To test this hypothesis, we will use Electrochemical Impedance Spectroscopy (EIS) and Nuclear Magnetic Resonance (NMR) techniques to evaluate the ionic conductivity of xylem fibers with and without a supporting electrolyte solution. By comparing the results, we will determine the efficacy of using a supporting electrolyte solution to enhance the ionic conductivity of xylem fibers and characterize the results of different electrolytes used. The findings of this study will contribute to a better understanding of the ionic transport system in plants and have potential applications in developing advanced biomimetic materials that can mimic the ionic transport properties of xylem fibers.</p>
9	Zachary Iton	California Institute of Technology	<p>Water Vapor Induced Superionic Conductivity in ZnPS₃</p> <p>Next-generation batteries based on sustainable divalent working ions have the potential to improve the performance, safety, and capacity of current battery systems. Development of such multivalent ion batteries is hindered by a lack of understanding of multivalent ionics in solids. For instance, multivalent ionic transport was assumed to be correlated with electronic transport, however, we have shown that Zn²⁺ can conduct in electronically insulating ZnPS₃ with a low activation energy of 350 meV. The conductivity, however, was also low. Here, we show that exposure of ZnPS₃ to different relative humidity environments results in room temperature conductivity increases of several orders of magnitude, reaching as high as 1.44 mS/cm without decomposition or structural changes. We utilize several electrochemical methods to confirm that both Zn²⁺ and H⁺ act as charge carriers. The contribution from Zn²⁺ to the conductivity in water vapor exposed ZnPS₃ is extremely high—representing superionic Zn²⁺ conduction. We find that it is possible to enhance multivalent ion conduction in electronically-insulating solids as a result of water absorption, and highlight the importance of ensuring that increased conductivity in water vapor exposed multivalent ion systems is in fact due to mobile multivalent ions and not H⁺.</p>
10	Jack Lang	University of California, Irvine	<p>Understanding Oxygen Transport in PTLs Using X-ray Computed Tomography</p> <p>Sintered and felt porous transport layers (PTLs) are commonly used in PEM electrolysis. Oxygen distribution in each type of PTL can be investigated at different current densities through operando X-ray computed tomography (CT) experiments. The results from these scans can show how oxygen transport compares between the two types of PTLs. Important morphological data such as porosity and pore size distribution can be extracted from these scans as well.</p>

11	Brian Lee	California Institute of Technology	<p>A Mg-In Alloy Interphase Suppresses Dendrites in Mg Metal Anodes</p> <p>Mg metal batteries have attracted much attention as an alternative to Li-ion technology due to Mg metal's high abundance and volumetric capacity. Reports suggested that Mg is less prone to dendritic growth compared to Li, improving the safety and long-term cyclability of Mg metal batteries. However, upon repeated cycling, heterogeneous growth of Mg is still observed in literature, causing cell shorting and capacity loss. We present a Mg-In alloy interphase to suppress heterogeneous Mg growth. With the alloy-coated Mg electrodes, a significant decrease in the heterogeneous Mg deposits formed on the surface is observed. The change in the deposition morphology results in a longer cell cycling lifetime before the cell shorts. We also present various <i>ex-situ</i> characterizations to study the mechanism of the morphology change. The system serves as a proof-of-concept for using alloy-based interphases to minimize heterogeneous metal deposition upon reduction, which can also be broadly applied to other metal anodes such as Li.</p>
12	Yin-Chen Lin	University of California, Santa Barbara	<p>Voltage-Calibrated, Finely Tunable Protein Assembly</p> <p>Neuronally triggered phosphorylation monotonically and cyclably drives the assembly of reflectin proteins, resulting in the fine-tuning of colors reflected from specialized skin cells in squid for camouflage and communication. Here we demonstrate for the first time that electrochemical reduction, which is used as a surrogate for phosphorylation-mediated charge neutralization, enables finely tunable and reversible control of the rate and size of reflectin assembly through a voltage-calibrated mechanism. This process is highly similar to the aforementioned physiological behavior. Electrochemically driven <i>in-situ</i> dynamic light scattering, circular dichroism, and UV absorbance spectroscopies were used to drive and simultaneously analyze the evolution of conformational transitions and assembly. Calibration of reflectin assembly with voltage is partly attributed to the protein's dynamic arrest property, which has previously been demonstrated to play a role in calibrating the correlation between the extent of neuronally triggered charge neutralization and the resulting fine-tuning of color in the biological system. The findings of this study open a new perspective on electrical regulation and simultaneous observation of reflectin assembly and more broadly provides access to manipulate, observe, and electrically control the formation of intermediates and conformational dynamics in other macromolecular systems.</p>

13	Emily Marquez	California State University, Long Beach	<p>Probing Adsorbate-Induced Effects During Hydrogen and CO₂ Reactions with pH on Au Surfaces</p> <p>We report on electrochemical analysis and stress measurements of hydrogen and CO₂ reactions on Au surfaces in aqueous solutions with different pHs. Interestingly, surface activation and catalysis of hydrogen and CO₂ on transition metal surfaces show preferential reactivity on select surfaces under controlled solution conditions. Here, we explore the reaction mechanism and early stages of catalysts activation during hydrogen and CO₂ reactions on well-defined Au surfaces under controlled solution conditions, i.e. pH and anion species. Well-defined Au surfaces are prepared using evaporation and atomic layer electrochemical deposition. Electrochemical analysis shows changes in surface reactivity toward HER and CO₂ reduction as the surface composition and structure is altered. Our stress analysis shows that hydrogen activation on surfaces causes a compressive stress, that can be used as a signature for activity toward hydrogen reactions. Interestingly, in-situ stress measurements of Au surfaces do not show surface activation of hydrogen even at low pHs. However, our analysis reveals stress responses corresponding to CO₂ interaction with Au surface. The CO₂ stress responses are evident at ca. 0.4–0 V vs. RHE. The stress response is different from what is observed for hydrogen activation on surfaces. We also use rate dependence of stress response to identify surface charge and flux effects of primary activation steps. We particularly show that CO₂ related features are flux dependent and are most dominant at pH = 7. Our studies show that at higher pHs water is involved in the hydrogen reactions even on Pt surfaces. Features which are likely due to water interactions are also observed on Au surfaces, however in the presence of CO₂, features which evolve with scan rate and cycling appear in stress analysis. We will discuss the origins of CO₂ related features on Au surfaces. These studies will provide insight into activity and selectivity descriptors for CO₂ reduction reactions on transition metal surfaces in aqueous media.</p>
14	Eloise Masquelier	University of California, Santa Barbara	<p>Electrochemical Triggering and <i>In-situ</i> Optical Interrogation of Tau Peptide Folding and Assembly</p> <p>Tau protein's reversible assembly and binding of microtubules in brain neurons are regulated by charge-neutralizing phosphorylation, while its hyperphosphorylation drives irreversible formation of cytotoxic filaments associated with neurodegenerative diseases. Under physiological conditions, tau is intrinsically disordered, remarkably stable and requires the use of aggregation inducers such as heparin to trigger its assembly <i>in vitro</i>. We analyzed K18, a core peptide of tau, using a newly developed method that combines heterogeneous electrochemistry with <i>in-situ</i> UV absorbance, circular dichroism and dynamic light scattering spectroscopies, to dynamically follow its conformational transitions and assembly. Electroreduction of lysine residues in K18 peptide acts as a surrogate for charge neutralization by phosphorylation, inducing rapid formation of beta-rich filaments without the need for preformed seeds or polyanions. Specific assembly conditions (electrochemical potential-, time- and salt concentration- dependent) reveal divergent trajectories of K18 assembly that parallel tau's <i>in vivo</i> behaviors. Advantages of the method include (i) the ability to control, kinetically resolve, and potentially isolate, never-before-seen intermediates in the process of folding and assembly; (ii) the ability to conduct such analyses without the need for aggregation inducers; and (iii) the ability to develop assays for potential effectors and regulators that can direct the trajectory of amyloid-related assembly.</p>

15	Magnolia Pak	University of California, Irvine	<p>High Temperature (150–300 °C) Polymer Electrolyte Membrane Reversible Fuel Cell</p> <p>Energy storage and conversion are critical components of the transition from fossil fuels to renewable energy. Reversible fuel cells (RFCs) are one possible solution that is well suited for applications requiring minimal storage volume and equivalent charge/discharge cycles. In this exploratory work, we propose the application of high temperature (150–300 °C) polymer electrolyte membrane (PEM) systems in RFC applications.</p>
16	Eshaan Patheria	California Institute of Technology	<p>Multielectron Transition Metal and Anion Redox in Lithium-Rich Iron Sulfides</p> <p>Li-ion battery cathode materials that invoke multielectron transition metal and anion redox can achieve higher energy densities than commercial state-of-the-art single-electron redox materials like $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ (NMC811) and LiFePO_4, which have energy densities of ~ 950 and $\sim 580 \text{ Wh}\cdot\text{kg}^{-1}$, respectively. LiFePO_4, despite low energy density, is growing in commercial production due to unconstrained supply chains of Fe and P compared to Co and Ni. However, higher energy density Fe-based cathodes are required to achieve widespread ($\sim 10^2 \text{ TWh}$) commercial deployment. Here, we substitute Li_2FeS_2 to develop a new family of materials that invokes multielectron redox <i>via</i> $\text{Fe}^{2+/3+}$ and $2\text{S}^{2-}/(\text{S}_2)^{2-}$ redox couples. We achieve high energy densities $>1,100 \text{ Wh}\cdot\text{kg}^{-1}$ with $>99\%$ Coulombic efficiency, surpassing state-of-the-art NMC811. The choice of sulfides is vital to the reversibility. By substituting Li_2FeS_2, we show that we can tune multielectron redox charge transfer dynamics between Fe and S. Our findings highlight the coupled roles of Fe and S throughout the multielectron redox mechanism, showing that local electron density redistribution between Fe and S sustains global multielectron redox in the materials. Our insights on the multielectron redox reaction mechanisms establishes new structure-property relationships about the coupled roles of metal d and anion p states in multielectron redox materials at large.</p>
17	Hunter Pauker	University of California, Irvine	<p>Correlated Computed Properties and Free Energies for Catalyst Optimization</p> <p>Optimizing matter <i>via</i> computational chemistry promises speed and chemical insight. To explore the possibility of quantitatively relating catalytic free energy surfaces (FES) to composition, we have computed (using DFT improved by select CCSD(T) calculations) FESs for two candidate reactions and material descriptors for modular catalyst components. pH- and potential-dependent microkinetic models generated Tafel plots. The electrocatalytic reduction of CO_2 to formate was studied using CpX complexes of first-row transition metals. A surprising variety in the FESs for this family was observed, and predicted H/D KIE values can be used as a rubric to interpret new experiments. Linear algebra tools applied to the FESs identify all free energy relationships, leaving effectively three degrees of freedom for catalyst optimization. Methane oxidation was studied using Ir(III) complexes and ligands that varied in their σ, π, steric properties and charge. Regression models related these properties to DFT-derived FESs and predicted the FESs of catalysts not yet simulated, identifying promising compositions to be added to the training set. As the training set for establishing these relationships grew, turnover frequencies plateaued. The limitations of this method were better understood and the combination of ligand properties for minimizing the C–H cleavage barrier while preventing unwanted oxidation was identified.</p>

18	Brian Roehrich	University of California, Santa Barbara	<p>Rapid Interrogation of Aptamer-Based Biosensors using Impedance Spectroscopy</p> <p>Electrochemical aptamer-based (EAB) biosensors are capable of continuously measuring molecular concentrations, <i>in vivo</i>. They rely on a target-sensing sequence of DNA (an aptamer), which is bound to an electrode and tagged with an electrochemical reporter. Binding of the specific target molecule (for example, a drug, metabolite, or protein) induces a conformational change in the aptamer, altering the distance between the redox reporter and the electrode surface. This phenomenon is used to generate an electrochemical response which depends on the concentration of the target molecule. In this poster, I will display our recent work on using electrochemical impedance spectroscopy (EIS) as a way to rapidly interrogate EAB sensors. EIS offers faster time resolution when compared to comparable voltammetric methods, and allows for calibration-free sensor operation, even in the living body.</p>
19	Hanson Wang	University of California, Irvine	<p>Novel Support Materials for Durable ORR Catalysts</p> <p>Carbonaceous materials are widely used as supports for platinum-based oxygen reduction reaction (ORR) catalysts that are prevalent in proton exchange membrane fuel cells (PEMFC). In particular, a variety of carbon blacks are popular due to factors such as commercial availability and high surface area. However, as mobile applications of PEMFCs shift more towards heavy-duty usage, durability of the supports has become an important criterion when evaluating materials. Carbon support corrosion can lead to Pt detachment and agglomeration, both of which decrease the electrochemically active surface area of the catalyst. Recently, nitrogen-doping of carbon supports has shown promising results towards stability in ORR operating conditions¹. Moreover, spheroidal particles have the lowest geometric surface area to volume ratio of three-dimensional materials. In this work, we will present a set of nitrogen-doped carbon nanosphere supports obtained <i>via</i> a one-pot colloidal synthesis and then decorated with Pt nanoparticles for ORR catalysis (Pt/NCS). The nitrogen-doped supports are monodisperse, contain a mesoporous pore structure, and show a higher level of bulk graphitization than commercial carbon blacks. Our work also elucidates how differences in certain nitrogen moieties on the carbon support's surface impact catalytic activity. The Pt/NCS catalysts exhibit similar mass activity and improved specific activity in RDE measurements for ORR compared to a commercial platinum-carbon catalyst at similar Pt weight loading.</p>
20	Stephanie Wang	University of California, Santa Barbara	<p>Towards Electrochemical Biosensors: Optimization of Enzyme Loading in Conductive Polymer Thin-Films</p> <p>Hybrid nanomaterial/biomolecule composites are becoming ubiquitous in the landscape of biosensors architectures. Enzyme-embedded conductive polymer thin films (ECP-TFs), in particular, enable fast and sensitive determination of biologically active compounds, while maintaining biological functionality. Our work focuses on the interplay between enzyme loading and device performance for the development of more effective and long-lived electrochemical biosensors. Here, we characterize the maximum loading capacity of enzymes into ECP-TFs, the activity per enzyme load, and the conductivity per enzyme load using glucose oxidase and PEDOT:PSS as our enzyme and polymer, respectively. We hypothesize that there might be an ideal "range" of composition to achieve maximum device performance. Our findings show that while the polymer conductivity remains constant even at ultra-high enzyme loading, leaching and maximum enzymatic activity are sensitive to the relative enzyme load.</p>

21	Yiheng Zhao	University of California, Irvine	Influence of Microstructure and Sodium Doping on Charge Transport in High Entropy Oxides High entropy oxides (HEOs) contain-five or more oxide components and form a single phase after processing. Doping HEOs with alkali metals, such as lithium and sodium, significantly-increases their electrical conductivity, indicating that -HEOs are promising for energy storage and battery applications. However, the mechanisms behind the reduction in charge transfer resistance, and the role of composition and microstructure, is not fully understood. Here we investigate the role of Na doping and microstructure on the electrical behavior of bulk sintered $(\text{Co,Cu,Mg,Ni,Zn})_{(1-x)}\text{Na}_x\text{O}$. Activation energies obtained from impedance measurements at elevated temperatures were used to elucidate the primary mechanisms contributing to charge transport in the grain bulk and grain boundaries. Results demonstrate that highly doped samples exhibit easier transport at the grain boundaries.
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7 Session Talks

7.1 Session 1A: Electrochemical Sensors

Chair: Adam Grosvirt-Dramen

Location: ISEB 1310

11:00 - 11:20 a.m.

On the Disinfection of Electrochemical-Aptamer Based Sensors

Julia Chung

University of California, Santa Barbara

Electrochemical aptamer-based (EAB) sensors enable the continuous, real-time detection of drugs and metabolite targets in the body. This platform is simultaneously (1) general, being independent of the chemical or enzymatic reactivity of its target; (2) continuous and lag-free; and (3) selective enough to deploy *in-situ* in the living body. Accordingly, much interest surrounds EAB sensors as a candidate technology for biomedical research and the diagnosis, treatment, and monitoring of disease. However, utilizing these devices in long-duration animal models, much less in human patients, requires that they be free of any significant pathogen load. Thus motivated, we have characterized the compatibility of EAB sensors with standard sterilization and high-level disinfection techniques. In doing so, we find that, while many cleaning protocols lead to significant sensor degradation, treatment with CIDEX OPA (0.55% ortho-phthalaldehyde) leads to effective disinfection without causing any detectable loss in sensor performance.

11:20 - 11:40 a.m.

Electrochemical Investigation of Enzyme Kinetics with an Unmediated, Unmodified Platinum Microelectrode

Connor Davis

University of California, Santa Barbara

Biosensors are an immensely popular electroanalytical technique, coupling biological specificity readily to a digital output in a miniaturizable format. Such systems can also be used to investigate the fundamental behavior of enzymes, describing the thermodynamics of their redox sensors and the kinetics of the reactions they drive. Both areas of interest have taken significant efforts to immobilize enzymes onto electrode surfaces, as it offers stability, reusability and potential unmediated communication with the active sites. However, immobilization has proven difficult to achieve universally, often altering the enzyme's structure and behavior.

Here, I show that an electrochemical investigation of glucose oxidase (GO_x) kinetics and thermodynamics parameters such as V_{max} and K_m can be done using an unmediated, unmodified platinum microelectrode which simplifies the experimental technique tremendously. This is achieved by analyzing picoamp per second increases in the chronoamperograms of hydrogen peroxide oxidation—the enzyme product. A comparison to the standard practice UV-Vis technique shows agreeable performance. Additionally, I explore the abilities and limitations of the electrochemical system to capture the effects from changing system parameters such as pH and oxygen concentration.

11:40 a.m. - 12:00 p.m.

Ethylene Sensing on an Electrodeposited Platinum Nanowire

Nicholas Humphrey

University of California, Irvine

Ethylene is a gas-phase molecule that controls plant ripening and is used in plastic manufacturing. At concentrations above 4% in air, however, this gas becomes explosive. By electrodepositing single platinum nanowires, we have created a gas sensor for the detection of ethylene and other olefins in air. The Joule-heating of the platinum nanowire creates a low-power and highly portable device that can detect ethylene in the single-ppm range. This talk will discuss the specificity of the sensor, the temperature dependence of the material, and the size effect of the nanowire on the response towards ethylene. A surface-scattering based mechanism for the chemiresistive response to ethylene will also be proposed.

12:00 - 12:20 p.m.

Investigating the Interplay between Applied Potential and Precision of Particle Sizing in Single-Entity Blocking Electrochemistry

Eric Liu

University of California, Santa Barbara

Blocking electrochemistry, a subfield of single-entity electrochemistry, enables in-situ sizing of a wide range of redox-inactive particles. This method uses the adsorptive impact of individual insulating particles on a microelectrode which decrease the electrochemical active surface area of the electrode. When there is an electroactive redox species in solution, each individual impacting particle results in discrete current drops, and the magnitude of the drop corresponds to the size of the particle blocking the electrode surface. One significant limitation of this technique is the “edge-effects.” This exists because of the inhomogeneous flux of the redox species’ diffusion due to increased mass transport onto the edge of the disk electrode surface. “Edge-effects” cause increased errors in size detection, and results in poor analytical precision. We demonstrate that moving away from where the system is operating under diffusional regime, and towards a kinetic regime by changing the applied potential increases the precision significantly. In addition, we demonstrate that this method of precision enhancement is not limited to spheres but also occurs for cubes. This work presents a novel methodology for edge effect mitigation of incredible simplicity, and shows its universality among different particle types.

7.2 Session 1B: Fuel Cells and Electrolyzers

Chair: Adam Zucconi

Location: ISEB 1200

11:00 - 11:20 a.m.

Modeling the Environment-Dependent Kinetics of Oxygen Reduction Reaction – a Continuum Model for Electric Double Layer

Masao Suzuki

University of California, Irvine

For proton exchange membrane fuel cells (PEMFCs) to achieve broad commercialization, kinetics of oxygen reduction reaction (ORR) needs to be better understood to improve the efficiency with minimized use of Pt-based electrocatalyst. The increasing demands of PEMFC-powered heavy-duty vehicles make this issue critical to meet the efficiency target (Cullen, Neyerlin et al. 2021). To understand ORR mechanisms, theoretical and experimental analyses have been conducted and explained the catalyst-dependent activity on single crystal catalysts in 0.1 M HClO₄ solution (Shibata, Inaba et al. 2022). Further studies are required to understand the effect of the electrolyte, which is experimentally reported (Kodama, Motobayashi et al. 2017) but not thoroughly understood yet. In this talk, we propose a multiscale continuum model to examine the effect of electrolyte concentration on ORR activity on Pt (111). After a model validation with the double layer capacity data (Pajkossy and Kolb 2001), the electrolyte concentration dependent ORR activity was analyzed. The model reproduced the experimental results by assuming the oxygen adsorption is limiting the rate, which can be attributed to the large energetic barrier for solvent reorganization (Limmer, Willard et al. 2013). In the presentation, the detail of the model, results, and the future direction will be explained.

11:20 - 11:40 a.m.

Understanding Oxygen Transport in PTLs Using X-ray Computed Tomography

Jack Lang

University of California, Irvine

Sintered and felt porous transport layers (PTLs) are commonly used in PEM electrolysis. Oxygen distribution in each type of PTL can be investigated at different current densities through operando X-ray computed tomography (CT) experiments. The results from these scans can show how oxygen transport compares between the two types of PTLs. Important morphological data such as porosity and pore size distribution can be extracted from these scans as well.

11:40 a.m. - 12:00 p.m.

Electrical behavior of multi-phase entropy-stabilized oxides

Aruto Meza

University of California, Irvine

Entropy-stabilized oxides (ESO) consist of five or more oxide components that form a random solid solution structure after processing. ESOs have garnered significant attention due to their interesting functional properties and expanded compositional space. For example, (Cu,Co,Mg,Ni,Zn)O shows promise for fuel cell and batteries components. Here we explore the role of processing, microstructure, and secondary phases on the electrical behavior of bulk (Co,Cu,Mg,Ni,Zn)O. Samples were consolidated using conventional sintering and heat treated at a range of temperatures and times to control the phase state. Temperature dependent impedance spectroscopy was used to investigate the role of microstructure on the electrical conductivity and activation energy for electrical transport. Electron and atomic force microscopy techniques were used to characterize the microstructure and tie it to the electrical behavior. Results show that processing and microstructure significantly influence the electrical behavior in (Co,Cu,Mg,Ni,Zn)O. Mechanisms governing the contribution of microstructure to electrical behavior will be discussed.

12:00 - 12:20 p.m.

Green Cement Manufacturing Using Electrolysis Technology

Hung-Ming Chang

University of California, Irvine

The production process of cement contributes to about 5% of industrial energy consumption and about 8% (8.2 Gton/year) of global CO₂ emissions. In conventional manufacturing process, calcination of CaCO₃ (limestone) is obtained in a kiln using energy input from non-renewable sources producing CaO. Carbon dioxide emission comes from both the decomposition reaction and from the combustion of the fuel necessary to provide heat to the system. As a result, about one ton of CO₂ is released for every ton of cement produced. Here we present a novel flow-through concept for Ca(OH)₂ production using a bipolar membrane flow-through reactor design. A single cell electrolyzer with serpentine flow field was used. A microfluidic spacer was introduced into the middle compartment between the two membranes and KCl electrolyte was supplied to remove the precipitate Ca(OH)₂. The presence of calcium hydroxide in the products is confirmed by FT-IR spectroscopy and XRD.

7.3 Session 2A: Batteries and Energy Storage I

Chair: Ethan Heffernan

Location: ISEB 1200

3:00 - 3:20 p.m.

Bridging the gap between pouch and coin cell electrochemical performance in lithium metal batteries

Charles Soulen

University of California, San Diego

While lithium metal anodes (LMA) are considered the “holy grail” of lithium-based anode materials, successful implementation remains elusive. One common, understudied problem with LMAs is the significant deviation in electrochemical performance between two common laboratory cell formats: coin and pouch cells. Generally, this discrepancy is blamed on the lower pressure provided by the coin cell relative to the pouch cell. Here, we report evidence that low pressure alone does not fully explain the Li plating behavior. Rather, the ring-like springs used in coin cells create an uneven pressure distribution within the cell, causing inhomogeneous Li plating and poor performance. Pouch cells, on the other hand, are commonly sandwiched between flat steel plates with rubber inserts, creating an even pressure distribution. By replacing the coin cell spring with an elastic rubber disc, a uniform pressure can be applied to the active materials, resulting in Li plating and cell performance more akin to pouch cells. Overall, this work represents the understudied intersection of electrochemistry and mechanics, both of which are necessary for improving device-level performance.

3:20 - 3:40 p.m.

Morphological Design of Silicon Anodes for Lithium-Ion Batteries

Sierra Gross

University of California, Irvine

Alloying type anodes for lithium-ion batteries, such as silicon, are desirable due to their high theoretical capacity; however large volume variations (~ 300 vol% for Si) during cycling can lead to mechanical degradation and loss of active material, resulting in an overall decline in electrochemical performance. Efforts to address these issues include the use of nanostructures and composites, which can require complex synthesis routes and decrease active material loading. An alternative route is to utilize thin coatings of active material on bicontinuous porous architectures. This allows for a balance of power and energy density, while simultaneously maintaining mechanical integrity. This project uses finite element analysis to study the mechanics of Si layers coated on spinodal, inverse opal, gyroid, and Schwartz primitive nickel backbones during expansion in order to explore the importance of surface curvature and morphology. This presentation highlights the promise of spinodal structures for alleviating expansion-induced mechanical degradation while also being amenable to scalable synthesis routes.

3:40 - 4:00 p.m.

Multielectron Transition Metal and Anion Redox in Lithium-rich Iron Sulfides

Eshaan Patheria

California Institute of Technology

Li-ion battery cathode materials that invoke multielectron transition metal and anion redox can achieve higher energy densities than commercial state-of-the-art single-electron redox materials like $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ (NMC811) and LiFePO_4 , which have energy densities of ~ 950 and ~ 580 $\text{Wh}\cdot\text{kg}^{-1}$, respectively. LiFePO_4 , despite low energy density, is growing in commercial production due to unconstrained supply chains of Fe and P compared to Co and Ni. However, higher energy density Fe-based cathodes are required to achieve widespread ($\sim 10^2$ TWh) commercial deployment.

Here, we substitute Li_2FeS_2 to develop a new family of materials that invokes multielectron redox *via* $\text{Fe}^{2+/3+}$ and $2\text{S}^{2-}/(\text{S}_2)^{2-}$ redox couples. We achieve high energy densities $>1,100$ $\text{Wh}\cdot\text{kg}^{-1}$ with $>99\%$ Coulombic efficiency, surpassing state-of-the-art NMC811. The choice of sulfides is vital to the reversibility.

By substituting Li_2FeS_2 , we show that we can tune multielectron redox charge transfer dynamics between Fe and S. Our findings highlight the coupled roles of Fe and S throughout the multielectron redox mechanism, showing that local electron density redistribution between Fe and S sustains global multielectron redox in the materials. Our insights on the multielectron redox reaction mechanisms establishes new structure-property relationships about the coupled roles of metal d and anion p states in multielectron redox materials at large.

7.4 Session 2B: Electrocatalysis I

Chair: Jack Lang

Location: ISEB 1010

3:00 - 3:20 p.m.

Nickel-Molybdenum HER and HOR Bifunctional Electrocatalyst obtained by Electrospinning

Giovanni Ferro

University of California, Irvine

The decarbonization of energy systems is driving the large-scale deployment of proton exchange membrane fuel cells and electrolyzers, which typically operate in acidic media and rely on scarce platinum group metals (PGM) to achieve industrially relevant reaction rates. The ability to operate these devices in an alkaline environment drastically changes the catalytic landscape of the electrochemical reactions involved. For example, in hydroxide exchange membrane fuel cells, the anodic hydrogen oxidation reaction (HOR) can limit cell efficiency to a degree comparable to the cathodic oxygen reduction reaction (ORR). Meanwhile, in alkaline electrolyzers the activity of Pt catalysts for the hydrogen evolution reaction (HER) drops to a level comparable to PGM free alternatives, making the search for these non-noble competitors particularly appealing. Here, we report on a novel PGM-free HER and HOR bifunctional catalyst developed by growing nickel-molybdenum alloy nanoparticles inside an in-house synthesized carbon fibrous support (NiMoCF). The catalyst was prepared by electrospinning of a solution containing polyacrylonitrile (PAN) and metal precursors, followed by pyrolysis in a reductive H₂ atmosphere. X-ray diffraction analysis shows that the NiMo alloy integrated within the carbon fibers is very similar to that obtained by Sadia et al., and shown to have exceptional HOR performance. The diffraction data suggests that the electrospinning process did not interfere with the mixing of the metal precursors, and that the reduction of the metal containing fibers at 550 °C led to the desired alloy. TEM imaging confirms the successful incorporation of the alloyed nanoparticles within the fibers, with virtually no particles coating the outer walls, and that a homogeneous distribution was achieved even at a high metal loading. The mesopore structure of the nanofibers can be tailored to facilitate efficient mass transport of the reactant to the NiMo sites, while keeping the sites anchored within the fiber, resulting in a highly active and durable catalyst. The technology described herein can be applied to other catalysis challenges, as it enables the scalable synthesis of conductive, high surface area and tunable electrocatalysts that feature the seamless incorporation of metallic nanoparticles within the support.

3:20 - 3:40 p.m.

Controlling the selectivity of CO₂ electroreduction through tuning the water content in nonaqueous electrolytes

Grace Chen

California Institute of Technology

Electrochemical reduction of CO₂ (CO₂RR) to value-added products provides a promising pathway for the production of fuels and commodity chemicals. Understanding the effect of the electrolyte and optimizing the electrolyte composition are important in tuning the selectivity of Cu-catalyzed CO₂RR. Herein, we study CO₂RR in acetonitrile using water as an exogenous proton donor. We investigate the effect of the activity of water on the product selectivity and the mechanistic pathway toward C₁ and C₂ products in acetonitrile. We hypothesize that by increasing the water activity in nonaqueous electrolytes, the adsorbed CO and H species will start to compete for active sites, thereby changing the rate of ethylene and methane production. This work demonstrates the ability of tuning water activity in Cu-catalyzed CO₂RR in nonaqueous electrolyte to alter the selectivity of CO, ethylene and methane formation and highlights the critical role of the electrolyte environment on product selectivity.

3:40 - 4:00 p.m.

Elucidating electrochemical nitrate and nitrite reduction over atomically-dispersed transition metal sites

Eamonn Murphy

University of California, Irvine

The electrochemical reduction of N-species to ammonia (NH_3) provides a carbon neutral pathway for NH_3 synthesis. However, the direct electrochemical activation and reduction of the insoluble and inert N_2 molecule remains unproven. As an alternative, the electrochemical nitrate reduction reaction (NO_3RR) offers a highly selective pathway for NH_3 synthesis. Nitrate (NO_3^-) is highly soluble in aqueous electrolytes at ambient conditions and has favorable adsorption energies compared to competing reactants such as H^+ , resulting in the NO_3RR to NH_3 being reported at high efficiencies, however, at relatively limited current densities. To make the levelized cost of NH_3 production more competitive with alternative approaches, large current densities and high efficiencies must simultaneously be realized. Here, building on our previous work (Murphy et al., *ACS Catal.* 2022, Murphy et al., *Submitted*) demonstrating the high selectivity of Fe-base materials for NO_3^- to NH_3 , we synthesize an active particle-active support system comprised of $\gamma\text{-Fe}_2\text{O}_3$ nanoparticles on single atom Fe-N-C, synergizing the activity of Fe at the nanoparticle and single atom level for ultrahigh NO_3RR activity maintaining -1.4 A/cm^2 at near 100% Faradaic efficiency to NH_3 over 24 hours, with *post-mortem* analysis showing the durability of the catalyst. Additionally, we evaluate the trade off between increased partial current density for ammonia and the reaction energy efficiency. This work highlights the effectiveness of active catalyst-active support systems for achieving NO_3RR to NH_3 at industrially relevant current densities.

7.5 Session 3A: Batteries and Energy Storage II

Chair: Adrien Stejer

Location: ISEB 1200

4:45 - 5:05 p.m.

Water Vapor Induced Superionic Conductivity in ZnPS₃

Zachery Iton

California Institute of Technology

Next-generation batteries based on sustainable divalent working ions have the potential to improve the performance, safety, and capacity of current battery systems. Development of such multivalent ion batteries is hindered by a lack of understanding of multivalent ionics in solids. For instance, multivalent ionic transport was assumed to be correlated with electronic transport, however, we have shown that Zn²⁺ can conduct in electronically insulating ZnPS₃ with a low activation energy of 350 meV. The conductivity, however, was also low. Here, we show that exposure of ZnPS₃ to different relative humidity environments results in room temperature conductivity increases of several orders of magnitude, reaching as high as 1.44 mS/cm without decomposition or structural changes. We utilize several electrochemical methods to confirm that both Zn²⁺ and H⁺ act as charge carriers. The contribution from Zn²⁺ to the conductivity in water vapor exposed ZnPS₃ is extremely high – representing superionic Zn²⁺ conduction. We find that it is possible to enhance multivalent ion conduction in electronically-insulating solids as a result of water absorption, and highlight the importance of ensuring that increased conductivity in water vapor exposed multivalent ion systems is in fact due to mobile multivalent ions and not H⁺.

5:05 - 5:25 p.m.

Tunable grain boundary conductivity in sodium doped high entropy oxides

Justin Cortez

University of California, Irvine

Concerns with the safety and sourcing of lithium-ion batteries have prompted significant research into sodium-based systems. High entropy oxides (HEO), which contain five or more oxide components in equimolar quantities, are ideal for battery applications due to their ability to accommodate a substantial quantity of mobile charge carriers (such as Na), while also demonstrating promising stability, conductivity, and capacity retention. Here we investigate the influence of sodium doping and microstructure on charge transport in bulk sintered (Cu,Co,Mg,Ni,Zn)_(1-x)Na_xO. We find that the conductivity increases with increasing dopant amount, up to 1.4·10⁻⁵ S cm⁻¹ at x=0.33. Much of this increase is attributed to the high grain boundary conductivity, which originates from a NaCoO₂ layered structure that forms in the grain boundaries during high temperature sintering. The relative contributions of the grain boundaries and the bulk to the charge transport are discussed, along with the ability to engineer grain boundaries in doped HEO materials.

5:25 - 5:45 p.m.

A Mg-In alloy interphase suppresses dendrites in Mg metal anodes

Brian Lee

California Institute of Technology

Mg metal batteries have attracted much attention as an alternative to Li-ion technology due to Mg metal's high abundance and volumetric capacity. Reports suggested that Mg is less prone to dendritic growth compared to Li, improving the safety and long-term cyclability of Mg metal batteries. However, upon repeated cycling, heterogeneous growth of Mg is still observed in literature, causing cell shorting and capacity loss. We present a Mg-In alloy interphase to suppress heterogeneous Mg growth. With the alloy-coated Mg electrodes, a significant decrease in the heterogeneous Mg deposits formed on the surface is observed. The change in the deposition morphology results in a longer cell cycling lifetime before the cell shorts. We also present various *ex-situ* characterizations to study the mechanism of the morphology change. The system serves as a proof-of-concept for using alloy-based interphases to minimize heterogeneous metal deposition upon reduction, which can also be broadly applied to other metal anodes such as Li.

7.6 Session 3B: Electrocatalysis II

Chair: Ben Ransom and Loki Chen

Location: ISEB 1010

4:45 - 5:05 p.m.

Electrochemical Carboxylation Using Carbon Dioxide as a Carbon Source

Rachel Baker

California Institute of Technology

Electrochemical carboxylation represents a sustainable method for the synthesis of valuable carboxylic acids and their derivatives. Unlike other common methods for carboxylic acid synthesis, which require stoichiometric oxidants or organometallic reagents, electrochemical carboxylation reactions generally operate under more mild conditions by using electricity as a driving force and carbon dioxide as a building block. To date, the electrochemical carboxylation literature has been focused on the incorporation of a single new carbon atom, from carbon dioxide, into a carbon chain. Incorporating several new atoms into the chain and forming multiple bonds in one pot through a technique such as alkene difunctionalization represents an exciting prospect. Tying together the theme of one-pot multiple bond formation with the investigation of new substrates for electrochemical carboxylation, we have envisioned a synthesis of carboxylic acids from aldehydes, alkenes, and carbon dioxide. Among all of the metal electrodes tested, cheap and abundant copper proved to be the best catalyst for the aldehyde/alkene coupling step. Using a radical-clock substrate, the radical nature of the aldehyde reduction intermediate has been supported. Ideally, with the incorporation of alcohol oxidation at the anode, this methodology would allow for the generation of a C₅-scaffold electrochemically entirely from carbon dioxide and water.

5:05 - 5:25 p.m.

Probing adsorbate-induced effects during hydrogen and CO₂ reactions with pH on Au surfaces

Emily Marquez

California State University, Long Beach

We report on electrochemical analysis and stress measurements of hydrogen and CO₂ reactions on Au surfaces in aqueous solutions with different pHs. Interestingly, surface activation and catalysis of hydrogen and CO₂ on transition metal surfaces show preferential reactivity on select surfaces under controlled solution conditions. Here, we explore the reaction mechanism and early stages of catalysts activation during hydrogen and CO₂ reactions on well-defined Au surfaces under controlled solution conditions, i.e. pH and anion species. Well-defined Au surfaces are prepared using evaporation and atomic layer electrochemical deposition. Electrochemical analysis shows changes in surface reactivity toward HER and CO₂ reduction as the surface composition and structure is altered. Our stress analysis shows that hydrogen activation on surfaces causes a compressive stress, that can be used as a signature for activity toward hydrogen reactions. Interestingly, in-situ stress measurements of Au surfaces do not show surface activation of hydrogen even at low pHs. However, our analysis reveals stress responses corresponding to CO₂ interaction with Au surface. The CO₂ stress responses are evident at ca. 0.4–0 V vs. RHE. The stress response is different from what is observed for hydrogen activation on surfaces. We also use rate dependence of stress response to identify surface charge and flux effects of primary activation steps. We particularly show that CO₂ related features are flux dependent and are most dominant at pH = 7. Our studies show that at higher pHs water is involved in the hydrogen reactions even on Pt surfaces. Features which are likely due to water interactions are also observed on Au surfaces, however in the presence of CO₂, features which evolve with scan rate and cycling appear in stress analysis. We will discuss the origins of CO₂ related features on Au surfaces. These studies will provide insight into activity and selectivity descriptors for CO₂ reduction reactions on transition metal surfaces in aqueous media.

5:25 - 5:45 p.m.

Model Nitrogen-Doped Carbon Nanosphere Supports for Platinum-Decorated Oxygen Reduction Reaction Catalysts

Hanson Wang

University of California, Irvine

Carbonaceous materials are widely used as supports for platinum-based oxygen reduction reaction (ORR) catalysts that are prevalent in proton exchange membrane fuel cells (PEMFC). In particular, a variety of carbon blacks are popular due to factors such as commercial availability and high surface area. However, as mobile applications of PEMFCs shift more towards heavy-duty usage, durability of the supports has become an important criterion when evaluating materials. Carbon support corrosion can lead to Pt detachment and agglomeration, both of which decrease the electrochemically active surface area of the catalyst. Recently, nitrogen-doping of carbon supports has shown promising results towards stability in ORR operating conditions¹. Moreover, spheroidal particles have the lowest geometric surface area to volume ratio of three-dimensional materials. In this work, we will present a set of nitrogen-doped carbon nanosphere supports obtained *via* a one-pot colloidal synthesis and then decorated with Pt nanoparticles for ORR catalysis (Pt/NCS). The nitrogen-doped supports are monodisperse, contain a mesoporous pore structure, and show a higher level of bulk graphitization than commercial carbon blacks. Our work also elucidates how differences in certain nitrogen moieties on the carbon support's surface impact catalytic activity. The Pt/NCS catalysts exhibit similar mass activity and improved specific activity in RDE measurements for ORR compared to a commercial platinum-carbon catalyst at similar Pt weight loading.

8 Acknowledgments

8.1 Conference Volunteers and Organizers

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8.2 ECS@UCI Board

Christopher Pantayatiwong Liu, President (cpliu1@uci.edu)

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