Live Session
Room Live - Session LI-TuM1

Tuesday Morning Live Session I: New Frontiers in Interfaces

Moderators: Ashleigh Baber, James Madison University, Erin Iski, U. Tulsa

10:00am **LI-TuM1-1 Welcome and Opening Remarks***, **Ashleigh Baber,*** James Madison University

Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

10:05am **LI-TuM1-2 Electrochemical Surface Science of Platinum***, **Marc Koper,*** Leiden University, Netherlands **INVITED**

Platinum is the most used electrocatalyst in electrochemical energy conversion devices such as fuel cells and electrolysers. In this talk I will highlight the recent work of my group on understanding the surface chemistry of platinum in an aqueous electrolyte, by combining single-crystal electrochemistry, density functional theory calculations, ultra-high-vacuum modeling, in situ spectroscopy and in situ electrochemical scanning tunneling microscopy. I will challenge some existing explanations and interpretations of platinum electrochemistry, and show the sometimes surprising surface disordering of platinum that happens at both positive (anodic) and negative (cathodic) potentials.

10:25am **LI-TuM1-6 Manipulating Electrochemical Reactions in Van Der Waals Heterostructures***, **Kwabena Bediako,*** University of California at Berkeley **INVITED**

Molecular-scale manipulation of electronic and ionic charge accumulation in materials is the backbone of electrochemical energy storage. Layered van der Waals (vdW) crystals are a diverse family of materials into which mobile ions can electrochemically intercalate into the interlamellar gaps of the host atomic lattice. The structural diversity of such materials enables the interfacial properties of composites to be optimized to improve ion intercalation for energy storage and electronic devices. However, the ability of heterolayers to modify intercalation reactions, and their role at the atomic level, are yet to be elucidated. In this talk I will discuss the electrointercalation of lithium at the level of individual atomic interfaces of dissimilar vdW layers. In this work, electrochemical devices based on vdW heterostructuresof stacked hexagonal boron nitride, graphene and molybdenum dichalcogenide (MoCh_2; Ch= S, Se) layers were constructed. Transmission electron microscopy, in situ magnetoresistance and optical spectroscopy techniques, as well as low-temperature quantum magneto-oscillation measurements and ab initio calculations, were used to resolve the intermediate stages of lithium intercalation at heterointerfaces. The formation of vdW heterointerfaces between graphene and MoCh_2 layers was found to result in a more than tenfold greater accumulation of charge in the metal dichalcogenidewhen compared to MoCh_2/MoCh_2homointerfaces, while enforcing a more negative intercalation potential than that of bulk Mo$Ch_2$by at least 0.5 V. Beyond energy storage, this combined experimental and computational methodology for manipulating and characterizing the electrochemical behavior of layered systems opens new pathways to control the charge density in two-dimensional electronic and optoelectronic devices.

10:45am **LI-TuM1-10 Scale-Up Manufacturing Processes for Powders: Pairing Powder Properties to Process***, **Arrelaine Dameron**, S. Moulton, J. DuMont , D. Lewis, T. Porcelli, R. Tracy,* Forge Nano **INVITED**

Control of surface phenomena by powder modification via atomic layer deposition (ALD) for a spectrum of technology applications has made its way to R&D literature. But commercial adoption of ALD powder modification has been perceived as slow and too expensive to consider as a realistic commercial process. Forge Nano has patented, constructed, and demonstrated a high throughput ALD powder manufacturing capability at commercial scale and is commercializing first markets with partners. The manufacturing capability for powder modification with ALD is unlocking new potential for lower-cost integration of ALD into products. We will discuss a cross-comparison of ALD manufacturing type to product application and scaling requirements. For the first time in history, a pathway for ALD-enhanced materials to be rapidly transitioned from lab-scale demonstration to commercial presentation is available for new product development. The scaleup process addresses the stepwise progression to validate engineering and materials requirements to meet the market price demands. We will demonstrate that ALD enabled materials are the state of the art. The manufacturing of consistent materials with ALD modification is a cost-competitive level and now possible. The future of material science and product development for operation at more demanding conditions is enabled by ALD for a variety of applications.

11:15am **LI-TuM1-16 Batteries at Work: Ambient Pressure Photoelectron Spectroscopy for Lithium Ion Batteries***, I. Källquist, F. Lindgren, M. Hahlin,* Uppsala University, Angstrom Laboratory, Sweden*; **Julia Maibach,*** Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany **INVITED**

Rechargeable ion batteries such as Li-ion batteries generally consist of a negative electrode, a positive electrode and an ion conducting electrolyte. Today, much of our knowledge about the interactions of these components at surfaces and interfaces comes from post mortem photoelectron spectroscopy (PES) analyses. For these types of measurements, pre-cycled battery electrodes are transferred to the PES instrument to be characterized in UHV conditions.

Using ambient pressure photoelectron spectroscopy (APPES), we now have the possibility to acquire more realistic information about the interplay of electrode and electrolyte since the experiments can be conducted at elevated pressures and with liquid electrolyte present. We will firstly present our contributions to characterizing Li-ion battery electrodes [1] and electrolytes [2] using APPES as a precondition to achieve reliable in-situ and operando studies on working batteries.

Secondly, we present our work on electrode/electrolyte interfaces to investigate changes in Galvani potential using *operando* APPES [3]. For Li-ion batteries, Galvani potential differences (i.e. the electrostatic potential difference between two phases in contact) play an important role for the reaction kinetics at the functional electrode/electrolyte interphases. However, due to lack of suitable measurement techniques, so far little is known about how the Galvani potential difference behaves during Li-ion battery operation. We will show our approach on measuring how a change in Galvani potential difference can be followed as a function of applied external voltage using *operando* APPES, even without direct access to the electrode/electrolyte interface.

[1] J. Maibach, C. Xu, S. K. Eriksson, J. Åhlund, T. Gustafsson, H. Siegbahn. H. Rensmo, K. Edström, M. Hahlin, Rev. Sci. Inst. 86 (2015), 044101.

[2] J. Maibach, I. Källquist, M. Andersson, S. Urpelainen, K. Edström, H. Rensmo, H. Siegbahn, M. Hahlin, Nature Comm. 10 (2019), 3080.

[3] F. Lindgren, I. Källquist, M.-T. Lee, A. Shavorskiy, K. Edström, H. Rensmo, L. Nyholm, J. Maibach, M. Hahlin, in preparation.

11:35am **LI-TuM1-20 In-Situ TEM Imaging of Nanoscale Reactions at Solid-Liquid-Gas Interfaces***, **Haimei Zheng,*** Lawrence Berkeley National Lab **INVITED**

Many chemical reactions involve the presence of solids, liquids and gases concurrently, for instance, heterogeneous catalysis, materials corrosion and others. Complex phenomena may occur at solid-liquid-gas interfaces. Direct monitoring the interfacial reactions at the nanoscale is significant for understanding the reaction mechanisms and developing strategies to control the reactions. By developing and applying liquid cell transmission electron microscopy (TEM), my group studies the dynamic nanoscale phenomena at solid-liquid-gas interfaces with high spatial and temporal resolution. In this talk, I will first show the observed accelerated etching of Au nanostructures with the presence of gas nanobubbles. Through tracking the evolution of local reaction profile and theoretical modeling, an understanding of the triple phase reactions and gas diffusion pathways at the interfaces is developed. I will also show that the solid-liquid-gas interfaces can play a critical role in mediating the oxidative etching by allowing the reduction reactions in a near distance. Future work on in situ TEM studies of the solid-liquid-gas interfaces and device applications will also be discussed.

11:55am **LI-TuM1-24 Molecular Processes in Ultra-High Vacuum between the Stars***, **Ewine van Dishoeck,*** Leiden University, The Netherlands **INVITED**

Stars and planets are born in the cold and ultra-tenuous clouds between the stars in the Milky Way. In spite of the extremely low temperatures and densities, a surprisingly rich and interesting chemistry occurs in these interstellar clouds, as evidenced by the detection of more than 200 different molecules. Water and a large variety of organic molecules are found, including simple sugars and high abundances of deuterated species. What are the molecular processes by which these molecules are formed and destroyed, both in the gas phase and on surfaces? And how do we calculate or measurerates that can be used in models of star-forming regions? Can these pre-biotic molecules end up on new planets and form the basis for life elsewhere in the universe? New data from the revolutionary Atacama Large Millimeter Array (ALMA) and the ESA-Rosetta mission to comet 67P will be presented.

12:15pm **LI-TuM1-28 Closing Remarks and Thank You's***, Erin Iski,* University of Tulsa

Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. We also look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

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