Surface Science
Room 305 - Session SS-WeA

Somorjai

Moderators: David Castner, University of Washington, **Prof. Jeong Park**, Korea Advanced Institute of Science and Technology (KAIST)

2:15pm **SS-WeA-1 Professor Somorjai's Impact on the Evolution of Surface Science**, ***Miquel Salmeron***, Lawrence Berkeley National Laboratory **INVITED**

The surface of materials usually exhibits unique chemical and electronic properties determined by their atomic structure, which is largely determined by their interaction with the external phases of vacuum, gas, liquid or solids. The current scientific foundation of the field of Surface Science was the result of the work of several Pioneers of which Professor Somorjai was a prominent one, who provided new concepts on the role of the surface structure that determine their properties. andthe development of new instruments. In this review I will highlight the evolution of surface science in the last 40 years, and the important role of the development of new instruments and the discoveries they brought, to the scientific and engineering communities.

2:45pm **SS-WeA-3 Professor Somorjai's Impact on my Journey from Single Crystals to Biomaterials**, ***David Castner***, Depts of Bioengineering & Chemical Engineering

Surface science plays an important role in a wide range of research and development areas such catalysis, biomaterials, microelectronics, clean energy and corrosion. The toolbox of surface scientist allows us to easily move across research topics and make significant impacts in both industrial and academic settings. The typical surface scientist is an expert in multiple techniques, surface modification, sample preparation/handling and instrumentation. We have all benefited from the significant and numerous advances that have occurred in the past 50 years in terms of improved instrumentation, introduction of new techniques and development of sophisticated data analysis methods, which has allowed us to perform detailed analysis of increasing complex samples. I am extremely grateful for the training I received during my PhD studies with Professor Somorjai as well as his continued mentorship and support throughout my career. This talk will discuss my adventures as a surface scientist starting from chemisorption and reactivity studies of small molecules on single crystal surfaces at UC Berkeley followed by industrial catalysis research at Chevron and eventually moving to biomedical surface analysis at the University of Washington. It has been an exciting journey and I will use it to provide some examples of the multidisciplinary nature of surface science embraced by Prof. Somorjai and his students, post-docs and staff. For example, comprehensive analysis of surfaces and surface immobilized molecules with modern surface science instrumentation provides an unprecedented level of detail about the immobilization process and the structure of the immobilized molecules. However, even with the advances that have been achieved with these powerful surface science techniques, there remain many significant challenges for surface scientist. These include characterizing the surface chemistry and structure of nanoparticles, determining the atomic level structure of complex molecules bound to surfaces, 3D imaging of samples, and improved sample preparation methods that maintain materials in a relevant state when using ultra-high vacuum-based analysis techniques.

3:00pm **SS-WeA-4 Surface Chemistry at the Sliding, Solid-Solid Interface**, ***Wilfred Tysoe***, University of Wiscosin-Milwaukee

Somorjai realized that the action of lubricants was inherently a surface science problem and, in 1995, was instrumental in launching Tribology Letters. The focus of the journal was to be on the science, rather than the engineering, of tribology, the study of friction and wear, and this is still its guiding principle today. Furthermore, the ultrahigh vacuum approach to understanding surface chemistry pioneered by Somorjai can be adapted to studying sliding-induced reaction pathways and this approach is illustrated here by studying a simple model tribochemical reaction consisting of the lubrication of copper by dialkyl disulfides. For example, this approach identifies a tribochemical reaction cycle, analogous to a catalytic reaction mechanisms, which includes shear-induced adsorbate decomposition and a mixing processes that causes adsorbates to be transported into the subsurface region to form a friction-reducing film. These model systems are sufficiently simple so that they are amenable to being analyzed using first-principle density-functional theory calculations that allow a deep understanding of the physical principles that underpin stress-induced reactions on surfaces to be obtained.

3:15pm **SS-WeA-5 Structural Evolution and Stability of Rh/TiO_2 Catalysts under CO_2 Hydrogenation Conditions**, ***Simon R Bare***, SLAC National Accelerator Laboratory; *Greg Barber,* Penn State University; *Xiaobo Chen, Judith Yang,* Brookhaven National Laboratory; *Robert Rioux,* Penn State University

At low temperatures (< 400°C), single atoms of Rh supported on rutile TiO_2 ($rTiO_2$) are responsible for the formation of CO during the reverse water gas shift (RWGS), while methane production is associated with the Rh-TiO_2 interface due to the observed correlation between methane formation rates and the volume-averaged Rh nanoparticle diameter.As the temperature is increased to >540°C, there is a notable increase in CO selectivity as the methane production rates tend towards zero.At 600°C and > 4 h time on stream, the catalytic behavior becomes completely agnostic to the initial Rh structure as well as weight loading, and the catalysts are highly selective for the RWGS reaction.Post-reaction HR-TEM image analysis confirms Rh nanoparticles crystallize/order during the reaction; at 400°C, most of the Rh particles are disordered, while at 600°C, they are more ordered. Infrared spectroscopy of CO adsorption on Rh nanoparticles supports the appearance of defined facets after annealing in nitrogen at high temperatures.will be referenced to the pioneering research of Gabor Somorjai in the 1980's where he showed the ability of Rh(111) surfaces and the Rh(111) terraces of stepped Rh single crystal surfaces to dissociate CO_2.

3:30pm **SS-WeA-6 Origins of Lipid Asymmetry in Supported Biomembranes**, ***Paul Cremer***, *Ruofei Wang, Ella Gregory,* Penn State University

Biological membranes show remarkable asymmetry in living systems. Phospholipids, such as phosphatidylethanolamine (PE) and phosphatidylserine (PS), primarily reside on the inner leaflet, while others, like phosphatidylcholine (PC) and sphingomyelin (SM), are more abundant on the outer leaflet. While maintaining this asymmetry in vivo requires significant energy from ATP-hydrolyzing enzymes, we show—using a novel lipid bilayer unzipping assay—that an uneven lipid distribution exists at equilibrium solely due to differences in the hydrogen-bonding environments between the leaflets. Specifically, a remarkable degree of asymmetry was generated using planar glass supports rich in hydrogen-bond acceptors that form stronger hydrogen bonds with PE and PS lipids than with water. Protein-coated substrates yielded nearly identical results. These findings have important implications for in vivo systems, where distinct hydrogen-bonding gradients naturally exist between the inner (cytoskeletal) and outer (glycocalyx) leaflets.

4:15pm **SS-WeA-9 Behavior of Cu-Pt Single-Atom Alloy Catalysts Under Realistic Conditions**, ***Francisco Zaera***, Dept. Chemistry **INVITED**

There has been some recent interest in the use of so-called single-atom catalysts, whereby one catalytic metal is isolated within a second to add a key but otherwise unavailable functionality, to control selectivity during the hydrogenation of organic reactants. We have recently shown that metal alloys consisting of Pt single atoms diluted within Cu nanoparticles selectively promote the hydrogenation of C=O bonds in unsaturated aldehydes, a reaction of interest in fine chemical manufacturing. Our rationale, that Cu surfaces may favor C=O over C=C hydrogenation steps with atomic hydrogen but may require Pt sites to promote the initial activation of molecular hydrogen, was corroborated by kinetic catalytic experiments. However, fundamental surface-science studies and quantum mechanics calculations showed a more nuanced picture. Specifically, IR titration experiments using carbon monoxide failed to identify Pt atoms accessible on the surface of the catalysts, suggesting that their catalytic contribution may involve indirect electronic changes on neighboring Cu atoms. Additional *in situ* x-ray absorption (XAS) data have indicated a preference for the Pt atoms to locate at the metal/support interface. DFT calculations also support the preference for the Pt atoms to be placed at the metal nanoparticle/silica boundary, and explain how they can still facilitate H_2 activation, remotely. These results have led us to reinterpret the way that single-atom alloy catalysts operate.

4:45pm **SS-WeA-11 Plasmonic Hot Carrier-Driven Catalytic and Photoelectrochemical Processes**, ***Jeong Y. Park***, Department of Chemistry, Republic of Korea

The detection of hot electrons and understanding the correlation between hot electron generation and surface phenomena are challenging questions in the surface science and catalysis community. The earlier works in Berkeley indicate hot electron flow generated on a gold thin film by photon

absorption (or internal photoemission) appears to be correlated with localized surface plasmon resonance. In addition, it has been found that the hot electron flux generated under photon absorption and exothermic chemical reaction is the major mediator of energy conversion process [1-3]. In this talk, I highlight the research direction to attempt to detect the surface plasmon driven hot carrier at the nanometer scale by using scanning probe microscopy. To detect and utilize the hot electron flows at the macroscale level, the metal-semiconductor nanodiodes were constructed. At the nanometer scale, we utilized photoconductive atomic force microscopy to observe photoinduced hot electrons on a triangular Au nanoprism on n-type TiO2 under incident light. This is the direct proof of the intrinsic relation between hot electrons and localized surface plasmon resonance. We observed surface plasmon induced hot hole by using the system of Au nanoprism on p-type GaN [4]. I will discuss the impact of hot carriers in the photocatalytic activity under photoelectrochemical water splitting by using Au-based plasmonic nanostructures [5] an AuPd bimetallic nanoparticles [6]. Plasmon-driven hot carriers provide new mechanistic insight into light–matter interactions at catalytic interfaces and offers a pathway toward designing highly efficient plasmonic energy conversion systems.

References

[1] J. Y. Park, L. R. Baker, and G. A. Somorjai, Chemical Reviews 115, 2781 (2015).

[2] H. Lee et al. Accounts of Chemical Research 55, 24, 3727 (2022).

[3] S. W. Lee et al. Surface Science Reports 76 100532 (2021).

[4] H. Lee et al. Advanced Science 7, 2001148 (2020).

[5] K. Song et al. ACS Energy Lett. 6, 4, 1333–1339 (2021).

[6] H. Park et al. Journal of the American Chemical Society 147, 39, 35913–35923 (2025).

5:00pm **SS-WeA-12 2D Ising Model for Enantiomer Adsorption on Achiral Surfaces: L- and D-Aspartic Acid on Cu(111)***, **Andrew Gellman**,* Carnegie Mellon University, USA

The 2D Ising model is well-formulated to address problems in adsorption thermodynamics. It is particularly well-suited to describing the adsorption isotherms predicting the surface enantiomeric excess, *ees*, observed during competitive co-adsorption of enantiomers onto achiral surfaces.

Herein, we make the direct one-to-one correspondence between the 2D Ising model Hamiltonian and the Hamiltonian used to describe competitive enantiomer adsorption on achiral surfaces. We then demonstrate that adsorption from racemic mixtures of enantiomers and adsorption of prochiral

molecules are directly analogous to the Ising model with no applied magnetic field, i.e., the enantiomeric excess on chiral surfaces can be predicted using Onsager's solution to the 2D Ising model. The implication is that enantiomeric purity on the surface can be achieved during equilibrium

exposure of prochiral compounds or racemic mixtures of enantiomers to achiral surfaces.

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