

Session Index

Session A2: Focus Session: Surface Chemistry and Catalysis I

Sponsoring Units: DCP

Chair: Graeme Henkelman, University of Texas - Austin

Room: 102

Monday, March 3, 2014 8:00AM - 8:36AM	A2.00001: Surface Chemistry of PdO(101) Invited Speaker: Jason Weaver
Monday, March 3, 2014 8:36AM - 8:48AM	A2.00002: Inelastic neutron scattering (INS) studies of hydrogen spillover on pure and Pd decorated metal oxides John Z. Larese , Sourav Adak , Nicholas Strange , Tilo Seydel , Chuck Sumner , Luke Daemen
Monday, March 3, 2014 8:48AM - 9:00AM	A2.00003: Interaction of H₂ with stoichiometric and O-rich RuO₂ (110) surfaces Yinying Wei , Umberto Martinez , Lutz Lammich , Flemming Besenbacher , Stefan Wendt
Monday, March 3, 2014 9:00AM - 9:12AM	A2.00004: Simple Molecules Adsorption Studies on Highly Epitaxial -Pure Phase- Delafossite CuFeO₂ Thin Films Alejandro Cabrera , Piero Ferrari , Toyanath Joshi , Pavel Borisov , David Lederman
Monday, March 3, 2014 9:12AM - 9:24AM	A2.00005: Computational Database of Metal-Oxide Surface Reactivities for Catalyst Design Michal Bajdich , Aleksandra Vojvodic , Jens K. Nørskov
Monday, March 3, 2014 9:24AM - 9:36AM	A2.00006: Density functional theory investigation of NO₂ and SO₂ adsorption on isolated and anatase-supported BaO clusters Mustafa Tek , Hande Ustunel , Daniele Toffoli
Monday, March 3, 2014 9:36AM - 9:48AM	A2.00007: <i>In-situ</i> NAP XPS studies of dissociative water adsorption on GaAs(100) surfaces Sylwia Ptasinska , Xueqiang Zhang
Monday, March 3, 2014 9:48AM - 10:24AM	A2.00008: Fundamental mechanistic studies in formic acid decomposition on transition metal surfaces Invited Speaker: Manos Mavrikakis
Monday, March 3, 2014 10:24AM - 10:36AM	A2.00009: Autocatalytic dissociation of water at stepped transition metal surfaces Rengin Pekoez , Swenja Woerner , Luca M. Ghiringhelli , Davide Donadio
Monday, March 3, 2014 10:36AM - 10:48AM	A2.00010: Trimethyltin Mediated Formation of Covalent Gold-Carbon Bonds Arunabh Batra , G. Kladnik , J. Meisner , M. Steigerwald , C. Nuckolls , D. Cvetko , A. Morgante , L. Venkataraman
Monday, March 3, 2014 10:48AM - 11:00AM	A2.00011: Epicalysis: Bending the third principle of catalysis Daniel Sheehan

Session Index

Session D1: Focus Session: Surface Chemistry and Catalysis II

Sponsoring Units: DCP

Chair: Charlie Sykes, Tufts University

Room: 103/105

Monday, March 3, 2014 2:30PM - 2:42PM	D1.00001: Plyler Prize and APS Fellow Introductions Gilbert Nathanson
Monday, March 3, 2014 2:42PM - 3:18PM	D1.00002: Earle K. Plyler Prize: Probing the Structural Evolution and Size-Dependent Reactivity of Gold Clusters by Photoelectron Spectroscopy Invited Speaker: Lai-Sheng Wang
Monday, March 3, 2014 3:18PM - 3:30PM	D1.00003: Understanding the Composition and Reactivity of Au/Cu Electrocatalyst Nanoparticles in Solution Using Highly Accurate Reactive Potentials Nongnuch Artrith , Alexie Kolpak
Monday, March 3, 2014 3:30PM - 3:42PM	D1.00004: Density Functional Theory Investigation of Adsorption Properties of CO, CO₂ and H₂O on γ-Al₂O₃ Supported Pt Clusters Mehmet Gokhan Sensoy , Hande Ustunel , Daniele Toffoli
Monday, March 3, 2014 3:42PM - 4:18PM	D1.00005: Correlating structure and function for nanoparticle catalysts Invited Speaker: Graeme Henkelman
Monday, March 3, 2014 4:18PM - 4:30PM	D1.00006: Catalytic Properties of Graphene-Supported Pt₁₃ Nanoclusters Ioanna Fampiou , Ashwin Ramasubramaniam
Monday, March 3, 2014 4:30PM - 4:42PM	D1.00007: Unexpected carboxylate like CO adsorption at the Sr₂Ru₂O₇ (001) surface Marcel Hieckel , Florian Mittendorfer , Josef Redinger , Bernhard Stoeger , Zhiming Wang , Michael Schmid , Ulrike Diebold
Monday, March 3, 2014 4:42PM - 4:54PM	D1.00008: Theoretical Study of Chemisorption on Nickel and Palladium Clusters Ajit Hira , Jose Pacheco , Danelle Jaramillo , Frank Naranjo
Monday, March 3, 2014 4:54PM - 5:06PM	D1.00009: Quantum Monte Carlo Calculations of Pt Nanoclusters and (111) Surface William Parker , Anouar Benali , Luke Shulenburg , Jeongnim Kim , Nichols Romero , Jeffrey Greeley
Monday, March 3, 2014 5:06PM - 5:18PM	D1.00010: Morphology and the Catalytic Activity of Pd Nanoparticles on TiO₂- and SrO-Terminated SrTiO₃ Nanocuboids Bor-Rong Chen , Cassandra George , Linhua Hu , Peter C. Stair , Kenneth R. Poeppelmeier , Richard P. Van Duyne , Yuyuan Lin , Michael J. Bedzyk
Monday, March 3, 2014 5:18PM - 5:30PM	D1.00011: Effective rate constants for nanostructured catalysts under diffusion limited conditions Shaun Hendy , Leila Rajabi

Session Index

Session F1: Focus Session: Surface Chemistry and Catalysis III

Sponsoring Units: DCP

Chair: Feng Tao, University of Notre Dame

Room: 103/105

Tuesday, March 4, 2014 8:00AM - 8:12AM	F1.00001: Parahydrogen Induced Polarization Reactions on Supported Metal Nanoparticle Catalysts Clifford Bowers , Ronghui Zhou , Wei Cheng , Luke Neal , Helena Hagelin-Weaver
Tuesday, March 4, 2014 8:12AM - 8:24AM	F1.00002: Nanosecond Dynamics in Pt Nanoparticles F.D. Vila , J.M. Moore , J.J. Rehr
Tuesday, March 4, 2014 8:24AM - 8:36AM	F1.00003: First principles molecular dynamics of metal/water interfaces under bias potential Luana Pedroza , Pedro Brandimarte , Alexandre Rocha , Marivi Fernandez-Serra
Tuesday, March 4, 2014 8:36AM - 9:12AM	F1.00004: Atom Specific Ultrafast Surface Chemistry using a Soft X-ray Laser Invited Speaker: Anders Nilsson
Tuesday, March 4, 2014 9:12AM - 9:24AM	F1.00005: Manipulation of Single Molecular Hydrogen in a Size-tunable Nanogap Hui Wang , Haiyan He , Shaowei Li , Wilson Ho , Ruqian Wu
Tuesday, March 4, 2014 9:24AM - 9:36AM	F1.00006: A model of the ideal molecular surface Bryan Henson , Laura Smilowitz
Tuesday, March 4, 2014 9:36AM - 9:48AM	F1.00007: Origin of unexpected attractive adsorbate-adsorbate interactions between negatively charged ions on Mg (0001) surfaces Su-Ting Cheng , Mira Todorova , J{"o}rg Neugebauer
Tuesday, March 4, 2014 9:48AM - 10:24AM	F1.00008: Multiscale Studies of Surface Chemistry of Catalysis: Au-Ag alloys Invited Speaker: Cynthia Friend
Tuesday, March 4, 2014 10:24AM - 10:36AM	F1.00009: Fe adsorption on the hematite (0001) and magnetite (111) surface Adam Kiejna , Tomasz Pabisiak
Tuesday, March 4, 2014 10:36AM - 10:48AM	F1.00010: Temperature programmed desorption of a binary gas mixture Nayeli Zuniga-Hansen , M. Mercedes Calbi
Tuesday, March 4, 2014 10:48AM - 11:00AM	F1.00011: Compton Scattering from Bulk and Surface of Water Wenjie Wang , Ivan Kuzmenko , David Vaknin

Session Index

Session J2: Focus Session: Surface Chemistry and Catalysis IV

Sponsoring Units: DCP

Chair: Jason Weaver, University of Florida

Room: 102

Tuesday, March 4, 2014 2:30PM - 2:42PM	J2.00001: Computational study of the ZGB model with a long-range interaction Chor-Hoi Chan , Per Arne Rikvold
Tuesday, March 4, 2014 2:42PM - 2:54PM	J2.00002: Benzene and Its Derivatives Adsorbed on Metal Surfaces: A Bag Full of Surprises Wei Liu , Matthias Scheffler , Alexandre Tkatchenko
Tuesday, March 4, 2014 2:54PM - 3:06PM	J2.00003: Selective self-assembly of molecular clusters with designed sizes on metal surfaces Jun Wang , Qing Li , Miguel Fuentes-Cabrera , Bobby G. Sumpter , Arthur P. Baddorf , Minghu Pan
Tuesday, March 4, 2014 3:06PM - 3:18PM	J2.00004: One Step Propylene Epoxidation by Size Selected Subnanometer Cluster Silver Catalysts: Structure-Function Relationships Resolved Through in Situ Studies Eric Tyo , Bing Yang , Janae DeBartolo , Sonke Seifert , Stefan Vajda
Tuesday, March 4, 2014 3:18PM - 3:30PM	J2.00005: Reaction-driven restructuring of Pt and Pd catalysts: In operando X-ray absorption spectroscopy study Annika Elsen , Ulrich Jung , Yuanyuan Li , Anatoly Frenkel , Ralph Nuzzo
Tuesday, March 4, 2014 3:30PM - 3:42PM	J2.00006: In-situ observation of sintering of Mono-metallic nanoparticles Vineetha Mukundan , Shiyao Shan , Jin Luo , Chuan-Jian Zhong , Oana Malis
Tuesday, March 4, 2014 3:42PM - 4:18PM	J2.00007: Exploration of surface chemistry and structure of catalysts under reaction condition and during catalysis with surface-sensitive in-situ techniques Invited Speaker: Franklin (Feng) Tao
Tuesday, March 4, 2014 4:18PM - 4:30PM	J2.00008: Acid-Base Interaction Induced Stability of Self-assembled Monolayer at Solid Interface Characterized by Sum Frequency Generation Spectroscopy He Zhu , Ali Dhinojwala
Tuesday, March 4, 2014 4:30PM - 4:42PM	J2.00009: First principles calculations of enthalpy and O-H stretching frequency of hydrogen-bonded acid-base complexes Mesfin Tsige , Ram Bhatta , Ali Dhinojwala
Tuesday, March 4, 2014 4:42PM - 4:54PM	J2.00010: Porous Particles: Controlling Molecular Diffusion within Metal-Organic Frameworks Ah-Young Jee , Melinda Sindoro , Steve Granick
Tuesday, March 4, 2014 4:54PM - 5:06PM	J2.00011: Manipulating the Band Structure of SrTiO₃ with Strain Darrell G. Schlom , Charles M. Brooks , Dagmar Chvostova , Vladimir Trepakov , Megan E. Holtz , Nik J. Podraza , Robert F. Berger , Lena F. Kourkoutis , Tassilo Heeg , Margitta Bernhagen , Reinhard Uecker , Juergen Schubert , Craig J. Fennie , Jeffrey B. Neaton , David A. Muller , Alexandr Dejneka
Tuesday, March 4, 2014 5:06PM - 5:18PM	J2.00012: Halide anion dependence of ionic surfactant adsorption in air/water interface Doseok Kim , Wenjie Wang , Woongmo Sung , Mingqi Ao , David Vaknin
Tuesday, March 4, 2014 5:18PM - 5:30PM	J2.00013: Interaction between M/CuO (M= Ti, V, Cr, Mn) as studied by X-ray Photoelectron Spectroscopy Anil Chourasia , Jacob Stahl

Session Index

Session L2: Focus Session: Surface Chemistry and Catalysis V

Sponsoring Units: DCP

Chair: Jill Millstone, University of Pittsburgh

Room: 102

Wednesday, March 5, 2014 8:00AM - 8:12AM	L2.00001: Structural Characterization of Mg/Al hydrotalcite-like Compounds and their Thermal Stability Shuhua Zhang , Siyuan Yang , Cheng Wang , Weijun Liu , Xiaodan Gu , Wenjun Gan , Xiaoyu Xue
Wednesday, March 5, 2014 8:12AM - 8:24AM	L2.00002: The Role of Cluster Size and Composition, the Nature of the Support / Interface on the Performance of gas Phase Heterogeneous Catalysts and Electrocatalysts Stefan Vajda
Wednesday, March 5, 2014 8:24AM - 8:36AM	L2.00003: Self-assembly of one-dimensional metal-organic nanoarchitectures on a surface Martina Capsoni , Agustin Schiffrin , Adam Shaw , Sarah Burke
Wednesday, March 5, 2014 8:36AM - 9:12AM	L2.00004: Unraveling the Role of Metal-Support Interactions in Heterogeneous Catalysis Invited Speaker: J.R. Schmidt
Wednesday, March 5, 2014 9:12AM - 9:24AM	L2.00005: Controlling Surface-Mediated Interactions at the Organic Semiconductor / Metal Interface Oliver Monti , Nahid Ilyas , Rocio Cortes-Rodriguez , Percy Zahl , Peter Sutter
Wednesday, March 5, 2014 9:24AM - 9:36AM	L2.00006: Trapping of Excited Electrons at the NaCl/Ag(100) Interface David Suich , Benjamin Caplins , Alex Shearer , Charles Harris
Wednesday, March 5, 2014 9:36AM - 9:48AM	L2.00007: NO_x Direct Decomposition: Potentially Enhanced Thermodynamics and Kinetics on Chemically Modified Ferroelectric Surfaces Arvin Kakekhani , Sohrab Ismail-Beigi
Wednesday, March 5, 2014 9:48AM - 10:24AM	L2.00008: First principles analysis of metal and oxide-metal interfacial catalysis for hydrogen production Invited Speaker: Jeffrey Greeley
Wednesday, March 5, 2014 10:24AM - 10:36AM	L2.00009: Spectroscopic Analysis of Ion Concentration Profile at Electrode/Electrolyte Interface by Interferometry David Moore , Ravi Saraf
Wednesday, March 5, 2014 10:36AM - 10:48AM	L2.00010: Density functional theory simulation of hydrogen-bonding vibrational densities of states at the quartz (101)-water interface and its relation to dissolution in aqueous solutions of ions Mark DelloStritto , James Kubicki , Jorge Sofu
Wednesday, March 5, 2014 10:48AM - 11:00AM	L2.00011: Directly Grafting Alkanethiol on Bare Si (111) by UV-assisted Photochemical Reaction Lo-Yueh Chang , Hung-Wei Shiu , Shangjr Gwo , Chia-Hao Chen

Session Index

Session Q2: Focus Session: Surface Chemistry and Catalysis VI

Sponsoring Units: DCP

Chair: J.R. Schmidt, University of Wisconsin-Madison

Room: 102

Wednesday, March 5, 2014 2:30PM - 3:06PM	Q2.00001: Ligand-Mediated Synthesis of Colloidal Nanoparticle Alloys Invited Speaker: Jill Millstone
Wednesday, March 5, 2014 3:06PM - 3:18PM	Q2.00002: The Double-edged Impact of Platinum Nano-Deposits on the Durability of Polymer Electrolyte Membranes --- A Theoretical Study Mohammad Javad Eslamibidgoli , Pierre-\Eric Alix Melchy , Ata Roudgar , Michael H. Eikerling
Wednesday, March 5, 2014 3:18PM - 3:30PM	Q2.00003: Computational modeling of the surface properties of uranium dioxide using hybrid DFT Megan Hoover , Raymond Atta-Fynn
Wednesday, March 5, 2014 3:30PM - 3:42PM	Q2.00004: Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of Mg₂MSO_x Saswata Bhattacharya , Sergey Levchenko , Luca Ghiringhelli , Matthias Scheffler
Wednesday, March 5, 2014 3:42PM - 3:54PM	Q2.00005: Density Functional Theory Studies of Sb(V) Oxyanion Adsorption on α-Al₂O₃ $\overline{110}$ surfaces Sai Kumar Ramadugu , Sara Mason
Wednesday, March 5, 2014 3:54PM - 4:06PM	Q2.00006: Artificial Photosystem I and II: Highly Selective solar fuels and tandem photocatalysis Yuchen Ding , Ignacio Castellanos , Logan Cerkovnik , Prashant Nagpal
Wednesday, March 5, 2014 4:06PM - 4:18PM	Q2.00007: K⁺-hydration in a low-energy two-dimensional wetting layer on the basal surface of muscovite Peter J. Feibelman
Wednesday, March 5, 2014 4:18PM - 4:54PM	Q2.00008: Conversion of solar into chemical energy on plasmonic metal nanostructures Invited Speaker: Suljo Linic
Wednesday, March 5, 2014 4:54PM - 5:06PM	Q2.00009: Impact of the vapour pressure of water on the equilibrium shape of ZnO nanoparticles: An ab-initio study Stephane Kenmoe , Mira Todorova , P. Ulrich Biedermann , Joerg Neugebauer
Wednesday, March 5, 2014 5:06PM - 5:18PM	Q2.00010: Fast diffusion of water nanodroplets on graphene --- surfing the waves Ming Ma , Angelos Michaelides , Gabriel Aeppli
Wednesday, March 5, 2014 5:18PM - 5:30PM	Q2.00011: Asymmetric Wettability Directs Leidenfrost Droplets Rebecca Agapov , Jonathan Boreyko , Dayrl Briggs , Bernadeta Srijanto , Scott Retterer , C. Patrick Collier , Nikolay Lavrik