

Elementary reaction steps in electrocatalysis: Theory meets Experiment

DFG Research Unit FOR1376

Workshop

October 28-31, 2012
Reisenburg

<http://www.uni-ulm.de/nawi/nawi-theochemfg/veranstaltungen/oktober-2012/workshop-home.html>

Schedule Sunday, October 28

14:00 - 18:30	<i>Arrival and registration</i>	
18:30 - 20:00	<i>Dinner</i>	
20:00 - 20:05	Axel Groß	<i>Opening remarks</i>
20:05 - 21:35	<i>Electrocatalysis</i>	
20:05 - 20:50	Elina Savinova	<i>Cooperative behavior on Pt microelectrode arrays</i>
20:50 - 21:35	Itai Panas	<i>Mechanistic Insights into Transition Metal Oxide Catalyzed Water Oxidation</i>

Monday, October 29

08:00 - 09:00	Breakfast	
09:00 - 12:30	<i>Electrocatalysis</i>	
09:00 - 09:45	Juan Feliu	<i>Some reflections on the understanding of oxygen reduction at Pt(111)</i>
09:45 - 10:30	Andrea Russell	<i>In situ XAS of core-shell electrocatalysts</i>
10:30 - 11:00	Coffee break	
11:00 - 11:45	Jean-Sebastien Filhol	<i>Rationalizing the Electrochemical Effects on Surfaces</i>
11:45 - 12:30	Jan Rossmeisl	<i>Towards atomic scale modelling of the electrochemical interface</i>
12:30 - 14:30	Lunch	
14:30 - 16:00	<i>Batteries/Solid State</i>	
14:30 - 15:15	Rotraut Merkle	<i>Oxygen exchange kinetics on perovskites - mechanistic insight from experiments and theory</i>
15:15 - 16:00	Kevin Leung	<i>First principles studies of electrochemical reactions at electrode/electrolyte interfaces in lithium ion batteries</i>
16:00 - 16:30	Coffee break	
16:30 - 18:00	<i>Electrocatalysis</i>	
16:30 - 17:00	Alexander Auer	<i>Modeling the ORR on Pt Nanoparticles</i>
17:00 - 17:30	Ludwig Kibler (P8)	<i>Electrochemical and electrocatalytic properties of PtRu single crystal alloys</i>
17:30 - 18:00	Jonathan Mueller (P1)	<i>Disentangling ligand and strain effects in RuPt ORR catalysts</i>
18:00 - 20:00	Dinner	
20:00 - 22:00	<i>Poster Session</i>	

Tuesday, October 30

08:00 - 09:00	Breakfast	
09:00 - 10:30	<i>Photoelectrocatalysis</i>	
09:00 - 09:45	Harald Oberhofer	<i>How do metal clusters split water? Towards a theoretical understanding of co-catalysts for water oxidation</i>
09:45 - 10:30	Alexander Shluger	<i>Modelling of electron and hole trapping at grain boundaries and interfaces in oxide nanostructures</i>
10:30 - 11:00	Coffee break	
11:00 - 12:30	<i>Electrocatalysis</i>	
11:00 - 11:45	Gary Attard	<i>Fundamental Studies of Metals and Polymers at Pt{hkl} Electrodes</i>
11:45 - 12:30	Ezequiel Leiva	<i>First-principles calculations of cyanide-modified Pt(111) surfaces</i>
12:30 - 14:30	Lunch	
14:30 - 18:00	<i>Electrocatalysis</i>	
14:30 - 15:00	Johannes Wiebe (P2)	<i>MD Simulation of Proton Discharge from Electrolyte Solutions</i>
15:00 - 15:30	Tanglaw Roman (P5)	<i>Properties of electrode-electrolyte interfaces studied from first principles</i>
15:30 - 16:00	Leandro Moreira de Campos Pinto (P3)	<i>Intermetallic compounds for hydrogen catalysis</i>
16:00 - 16:30	Coffee break	
16:30 - 17:15	Mikiel Sprik	<i>Redox reactions and the band structure of liquid water</i>
17:15 - 17:45	Renat Nazmutdinov	<i>Orbital overlap effects in heterogeneous electron transfer reactions: a quantum chemical approach</i>
18:30 - 21:00	Conference Dinner	
21:00 -	Social Event	

Wednesday, October 31

08:00 - 09:00	Breakfast	
09:00 - 12:30	<i>Electrocatalysis</i>	
09:00 - 09:45	Thomas Schmidt	<i>New electrocatalyst systems and old questions: Can we overcome current PEFC catalysis limits?</i>
09:45 - 10:30	Wolfgang Schuhmann	<i>Electrocatalysis Meets Scanning Electrochemical Microscopy</i>
10:30 - 11:00	Coffee break	
11:00 - 11:30	Fernanda Juarez (P6)	<i>Electronic anisotropy at silver stepped surfaces</i>
11:30 - 12:00	Jusys Zenonas (P4)	<i>Adsorption of C-1 molecules: electrochemical interface probed by IR spectroscopy at low temperatur</i>
12:00 - 12:30	Otavio Alves (P7)	<i>Electrochemical characterization of UHV-fabricated PtAu model electrodes monolayer islands vs surface alloy</i>
12:30 - 14:00	Lunch	
14:00	Departure	