

**Elementary reaction steps in electrocatalysis:  
Theory meets Experiment**

**DFG Research Unit FOR1376**

Program of the workshop

**Elementary reaction steps in electrocatalysis:  
Theory meets experiment**

Castle Reisenburg near Ulm/Germany

May 1-4, 2016



Organizer:

Axel Groß, Ulm University, Ulm/Germany

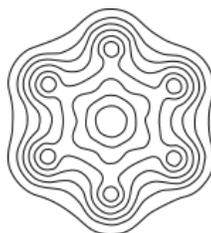
**Supported by:**

German Science Foundation (DFG) through Research Unit FOR 1376

Psi-k Network for Electronic Structure Calculations

Fonds der Chemischen Industrie

**DFG** Deutsche  
Forschungsgemeinschaft



**FCI**  
FONDS DER  
CHEMISCHEN  
INDUSTRIE



# Meeting programme

## Schedule Sunday, May 1, 2016

14:00 - 18:30	<i>Arrival and registration</i>	
18:30 - 20:00	<i>Dinner</i>	
20:00 - 20:45	Axel Groß	<i>Elementary reaction steps in electrocatalysis: Theory meets experiment</i>
20:45 - 21:30	Werner Tillmetz	<i>The importance of advanced electrocatalysts for fuel cell electric vehicles</i>

## Monday, May 2, 2016

08:00 - 09:00	Breakfast	
09:00 - 17:00	<i>Electro-catalysis</i>	
09:00 - 09:45	Enrique Herrero	<i>Formic acid electrocatalysis on platinum electrodes: Insights from theory and experiments</i>
09:45 - 10:30	Karen Chan	<i>Theoretical investigations of electrochemical CO<sub>2</sub> reduction</i>
10:30 - 11:00	Coffee break	
11:00 - 11:45	Jan Rossmeisl	<i>Special sites in electrocatalysis</i>
11:45 - 12:30	Nenad Markovic	<i>Energy and fuels from electrochemical interfaces</i>
12:30 - 14:30	Lunch	
14:30 - 15:15	Karsten Reuter	<i>First-principles photo-electrocatalysis beyond the computational hydrogen electrode</i>
15:15 - 16:00	Ifan Stephens	<i>Accelerating oxygen reduction towards H<sub>2</sub>O and H<sub>2</sub>O<sub>2</sub> on model alloy surfaces</i>
16:00 - 16:30	Coffee break	
16:30 - 17:00	Clotilde Cucinotta	<i>Towards a parameter-free theory of electrochemical phenomena at the nanoscale</i>
17:00 - 18:00		<i>Short presentation of posters</i>
18:00 - 20:00	Dinner	
20:00 - 22:00	<i>Poster Session</i>	

## Tuesday, May 3, 2016

08:00 - 09:00	Breakfast	
09:00 - 15:15	<i>Solid-liquid interfaces</i>	
09:00 - 09:45	Marie-Pierre Gaigeot	<i>Electrolytes at the (0001) alpha-quartz/water interface investigated by DFT-MD simulations</i>
09:45 - 10:30	Marialore Sulpizi	<i>Water orientation and hydrogen-bond structure at the fluorite/water interface</i>
10:30 - 11:00	Coffee break	
11:00 - 11:45	Mira Todorova	<i>Oxide stability and defect chemistry in an electrochemical environment: an ab initio perspective</i>
11:45 - 12:30	Richard G. Hennig	<i>Coupling of density-functional theory with continuum methods for solid/liquid interfaces and electrochemistry</i>
12:30 - 14:30	Lunch	
14:30 - 15:15	Olaf Magnussen	<i>Operando synchrotron X-ray scattering studies of electrochemical interfaces</i>
15:15 - 17:15	<i>Ionic Liquids</i>	
15:15 - 16:00	Alexei A. Kornyshev	<i>Unravelling charging dynamics in subnanometre pores: an overview</i>
16:00 - 16:30	Coffee break	
16:30 - 17:15	Dmitry Bedrov	<i>Ionic liquids at charged surfaces and inside nanoporous electrodes</i>
17:15 - 17:45	Sylvain Brimaud	<i>The reactivity of bimetallic electrodes at the atomic scale level: A challenge for the experimentalist</i>
17:45 - 18:15	Fernanda Juarez	<i>Electrocatalysis on stepped surfaces</i>
18:30 - 21:00	Conference Dinner	
21:00 -	Social Event	

## Wednesday, May 4, 2016

08:00 - 09:00	Breakfast	
09:00 - 12:30	<i>Energy storage</i>	
09:00 - 09:45	Helmut Baltruschat	<i>Bifunctional ORR and OER electrocatalysis for metal-oxygen batteries: Role of the catalyst</i>
09:45 - 10:30	Oleg Borodin	<i>Modelling lithium battery electrolytes and solid electrolytes interphases</i>
10:30 - 11:00	Coffee break	
11:00 - 11:45	Søren Dahl	<i>Electrochemistry at Haldor Topsøe</i>
11:45 - 12:15	Martin Korth	<i>Molecular materials for electrochemical energy storage: From computational screening to adaptive QM/MM simulations</i>
12:30 - 13:30	Lunch	
13:30	Departure	

# Abstracts

Sunday, May 1, 20:00

## **Elementary reaction steps in electrocatalysis: Theory meets experiment**

Axel Groß

Institute of Theoretical Chemistry, Ulm University, Ulm/Germany

In summer 2010, the German Science Foundation established the research unit FOR 1376 “Elementary reaction steps in electrocatalysis: Theory meets experiment”. DFG research units can run for two funding periods of three years each, and so the funding will end this year. The main goal of the research unit was to study elementary steps in electrocatalysis, however, the specific approach of this project was that it is not the experiment that will pave the way and determine the research direction, as is usually done in collaborative research programmes, but that theory will in fact take a leading role by defining important issues that need to be addressed for a better understanding of elementary reaction steps in electrocatalysis.

In this talk I will highlight some results that members of the research unit have been achieved during the last six years. In particular, I will try to address the question whether the research unit has achieved the goals that it had set six years ago.

Sunday, May 1, 20:45

## **The Importance of Advanced Electrocatalysts for Fuel Cell Electric Vehicles**

Werner Tillmetz

Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW), Ulm/Germany

For high performance, automotive fuel cells the electrocatalyst is the most crucial component. The electrocatalyst contributes to more than 50% to the cost of such a fuel cell stack. By improving the exchange current density, the efficiency can be improved, leading to an increased range of the vehicle. At the same time higher efficiency reduces the cooling requirements of the stack, which is also an challenging task in the development fuel cell vehicles.

Monday, May 2, 09:00

## **Formic acid electrocatalysis on platinum electrodes: Insights from theory and experiments**

Enrique Herrero

Instituto de Electroquímica, Universidad de Alicante, E-03080 Alicante, Spain

In this communication, recent results for the formic acid oxidation reaction will be reviewed, trying to establish the active species for the oxidation and the how to increase the catalytic activity on platinum electrodes. The combination of the electrochemical experiments conducted with different electrolytes, temperatures and pH results suggests that the relevant species in the oxidation process is an adsorbed formate molecule. The additional presence of adsorbed anions could catalyze the reaction. DFT calculations suggests that the active species is a formate molecule the C-H bond pointing towards the surface. The measured activation energies for the reaction suggests that anions or other adsorbed species may help positioning the molecule in the right direction and activating the reaction. This is the case of the electropositive adatoms on the surface, which, due to a partial negative charge facilitate the adsorption of formate in the right configuration. For these cases, the relevant parameter to estimate the catalytic enhancement for this reaction is the electronegativity of this adatom. It was found that adatoms with low electronegativity is a requirement for the catalytic enhancement. Experimental examples on those adatoms will be presented, corroborating the calculations.

Monday, May 2, 09:45

## Theoretical Investigations of Electrochemical CO<sub>2</sub> reduction

Karen Chan

Department of Chemical Engineering, Stanford University, Stanford, California/USA

The electroreduction of CO<sub>2</sub> has the potential to store energy from intermittent renewable sources and to produce carbon-neutral fuels and chemicals [1, 2]. In recent years, theoretical studies of CO<sub>2</sub> reduction have usually applied the computational hydrogen electrode model, which allows for the determination of the energies of reaction intermediates without explicitly treating the potential and the ions in solution [3]. This thermochemical approach has been shown to correlate well with experimental onset potentials [4, 5] and applied to computational screening of new catalysts [6]. However, an understanding of charge transfer barriers, kinetics, selectivity, and pH effects all require explicit consideration of solvent and charge. In this talk, we will discuss new developments in the explicit treatment of the electrochemical interface and their application to CO<sub>2</sub> reduction: barriers at constant potential [7], field effects, and C-C coupling [8].

References:

- [1] D.T. Whipple and P.J. Kenis, *J. Phys. Chem. Lett.* **1**, 3451 (2010).
- [2] C. Graves, S.D. Ebbesen, M. Mogensen, and K.S. Lackner, *Renewable and Sustainable Energy Reviews* **15**, 1 (2011).
- [3] J.K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J.R. Kitchin, T. Bligaard, H Jónsson, *J. Phys. Chem. B* **108**, 17886 (2004).
- [4] C. Shi, H.A. Hansen, A.C. Lausche, and J.K. Nørskov, *Phys. Chem. Chem. Phys.* **16**, 4720 (2014).
- [5] K.P. Kuhl, T. Hatsukade, E.R. Cave, D.N. Abram, J. Kibsgaard, and F. Thomas, *J. Am. Chem. Soc.* **136** 14107 (2014).
- [6] K. Chan, C. Tsai, H.A. Hansen, and J.K. Nørskov, *ChemCatChem* **6**, 1899 (2014).
- [7] K. Chan and J.K. Nørskov, *J. Phys. Chem. Lett.* **6**, 2663 (2015).
- [8] J.H. Montoya, C Shi, K. Chan, , and J.K. Nørskov, *J. Phys. Chem. Lett.* **6**, 2032 (2015).

Monday, May 2, 11:00

## **Special sites in electrocatalysis**

Jan Rossmeisl

University of Copenhagen

We need more efficient, selective and stable catalysts for future production of renewable fuels and chemicals. To obtain this we need to discover catalytic sites with special properties and find new design principles. I will give some examples on such special sites for energy conversion and formation of electrochemicals.

Monday, May 2, 11:45

## **Energy and fuels from electrochemical interfaces**

Nenad Markovic

Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

Advances in electrocatalysis at solid-liquid interfaces are vital for driving technological innovations that are needed to deliver reliable, affordable, and environmentally-friendly energy. Here, we highlight the key achievements in the development of new materials for efficient hydrogen and oxygen production in electrolyzers and, in the reverse, their utilization in fuel cells. Common descriptors for improving oxygen and hydrogen kinetics will be discussed. Links between aqueous- and organic-based environments will be established, encouraging “fuel cell” and “battery” community to move forward together.

Monday, May 2, 14:30

## **First-Principles Photo-Electrocatalysis beyond the Computational Hydrogen Electrode**

Karsten Reuter

Chair for Theoretical Chemistry and Catalysis Research Center  
Technische Universität München, D-85747 Garching/Germany

First-principles based computational modelling assumes an ever increasing role in understanding and partly already optimizing catalysts for photo-electrochemical reactions. The success of prevalent approaches like the computational hydrogen electrode (CHE) thereby relies largely on a numerical efficiency sufficiently high as to allow for large-scale screening of catalyst materials. Such efficiency arises out of well-chosen descriptors that ideally condense the mechanistic understanding of the ongoing catalytic reactions at the solid-liquid interface.

In recent years, there is increasing evidence that this understanding needs further scrutiny. Critical aspects in this respect are the neglect of solvation effects, the assumption of pathways that exclusively proceed via proton-coupled electron transfer steps, and the neglect of any kinetic limitations in the CHE approach. In this talk I will review our recent activities in addressing these issues with detailed first-principles based multiscale modeling approaches. Thereby, in particular embedding approaches both on the solid and the liquid side of the interface have the potential for a refined description without sacrificing computational efficiency.

Monday, May 2, 15:15

## Accelerating oxygen reduction towards $\text{H}_2\text{O}$ and $\text{H}_2\text{O}_2$ on model alloy surfaces

Ifan E. L. Stephens

Department of Physics, Technical University of Denmark, Lyngby  
Oxygen reduction is one of the most studied electrochemical reactions in the field of electrochemistry: it occurs in batteries, fuel cells, and enzymes in nature. I will present a series of model investigations, where we specifically aim to improve the catalysis of this ubiquitous reaction.

Most electrochemists would consider  $\text{H}_2\text{O}_2$  to be an unwanted side-product of oxygen reduction, to be avoided at all cost. However, it is a very useful chemical in its own right, with an annual global production exceeding 3 million tons. At present,  $\text{H}_2\text{O}_2$  is synthesised by the anthraquinone route, a complex, batch process, conducted in large scale facilities. The electrochemical production of  $\text{H}_2\text{O}_2$  would enable small scale production of hydrogen peroxide, closer to the point of consumption. The viability of the process is contingent on a catalyst that is active, stable and selective for  $\text{H}_2\text{O}_2$  production. We recently discovered a set of electrocatalysts that showed an unprecedented combination of all three of these desired properties: alloys of Pt, Ag or Pd with Hg<sup>1,2</sup>.

In low temperature fuel cells, high loadings of Pt are required to catalyse oxygen reduction to  $\text{H}_2\text{O}$ ; the short supply limits of Pt limits the extent to which fuel cell technology could be scaled up. The most widely used strategy to decrease the Pt loading is to alloy Pt with other metals. At our laboratory, we have developed a different class of catalyst for oxygen reduction: alloys of Pt with rare earths, such as Y or Gd. The strong interaction between Pt and the rare earth elements should make these compounds inherently resistant towards long term degradation via dealloying. We first demonstrated the high activity of Pt<sub>3</sub>Y and Pt<sub>5</sub>Gd on smooth bulk surfaces<sup>3-5</sup>. However, we have more recently shown that model, size-selected nanoparticles of these materials show equally superior performance<sup>6</sup>. Based on our detailed characterization of the catalysts, we deduced that the activity is due to a compressive strain imposed from the bulk onto the overlayer. On this basis, we conjectured that by changing the composition of the rare earth atom, we could modulate the activity. Lanthanide atoms tend to decrease in size with increased number of f-electrons. We harnessed this effect known as the lanthanide contraction to control both the activity and stability of these alloys<sup>7</sup>.

The catalysts under investigation include model-size selected nanoparticles, commercial high surface area catalysts, and well defined single crystals. We have probed these surfaces with electrochemical measurements, ultra-high vacuum based surface science methods, electron microscopy, synchrotron-based spectroscopy and density functional theory calculations.

1 Verdager-Casadevall, A., Deiana, D., Karamad, M., Siahrostami, S., Malacrida, P., Hansen, T. W., Rossmeisl, J., Chorkendorff, I. & Stephens, I. E. L. *Nano Lett.* 14, 1603, (2014).

2 Siahrostami, S., Verdager-Casadevall, A., Karamad, M. R., Deiana, D., Malacrida, P., Wickman, B., Escudero-Escribano, M., Paoli, E. A., Frydendal, R., Hansen, T. W., Chorkendorff, I., Stephens, I. E. L. & Rossmeisl, J. *Nature Materials* 12, 1137, (2013).

3 Greeley, J., Stephens, I. E. L., Bondarenko, A. S., Johansson, T. P., Hansen, H. A., Jaramillo, T. F., Rossmeisl, J., Chorkendorff, I. & Nørskov, J. K. *Nature Chemistry* 1, 552, (2009).

4 Stephens, I. E. L., Bondarenko, A. S., Grønby, U., Rossmeisl, J. & Chorkendorff, I. *Energy Environ. Sci.* 5, 6744, (2012).

5 Escudero-Escribano, M., Verdager-Casadevall, A., Malacrida, P., Grønby, U., Knudsen, B. P., Jepsen, A. K., Rossmeisl, J., Stephens, I. E. L. & Chorkendorff, I. *J. Am. Chem. Soc.* 134, 16476, (2012).

6 Hernandez-Fernandez, P., Masini, F., McCarthy, D. N., Strebler, C. E., Friebel, D., Deiana, D., Malacrida, P., Nierhoff, A., Bodin, A., Wise, A. M., Nielsen, J. H., Hansen, T. W., Nilsson, A., Stephens, I. E. L. & Chorkendorff, I. *Nature Chemistry* 6, 732, (2014).

7 Escudero-Escribano, M., Malacrida, P., Hansen, M. H., Vej-Hansen, U. G., Velazquez-Palenzuela, A., Tripkovic, V., Schitz, J., Rossmeisl, J., Stephens, I. E. L. & Chorkendorff, I. *Science* 352, 73, (2016)

Monday, May 2, 16:30

**Towards a parameter-free theory of electrochemical phenomena at the nanoscale**

Clotilde Cucinotta

Trinity College, Dublin, Ireland

Currently a comprehensive description of electrochemical conversion necessitates the modelling of both its electrical and chemical aspects, but none of the existing theoretical and computational methodologies can fully combine the two. In this talk it will be illustrated a possible way to integrate the effect of currents and bias in the modelling of atomic structure, dynamics and chemical transformation at electrified interfaces. This is achieved by combining the ability of the non-equilibrium Greens functions to deal with open boundary systems under current or bias with the ability of density functional theory based molecular dynamics to simulate chemical transformation. A preliminary implementation of the method and its application for the description of current induced atomic dynamics in a model system will be highlighted.

Tuesday, May 3, 09:00

## **Electrolytes at the (0001) alpha-quartz/water interface investigated by DFT-MD simulations**

Morgane Pfeiffer-Laplaud and Marie-Pierre Gaigeot

LAMBE UMR8587, Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement, Université d'Evry val d'Essonne, 91025 Evry/France

This talk is dedicated to probing the microscopic organization of silica-water interfaces including electrolytes by first principles DFT-based molecular dynamics simulations (DFT-MD). Ions from electrolytic solutions play key roles on interfacial water/mineral interfaces: their adsorption typically drives pollutant transport in groundwater, mineral dissolution, clay swelling, and electrolytes can strongly affect the binding of organic molecules because of competitive interactions. We will present our very recent DFT-MD simulations of electrolytic quartz-water interfaces (KCl, NaCl, NaI) in order to unravel the structural properties of these electrolytes at the interface between the quartz surface and liquid water. We provide some understanding on how the chemical properties and reactivity of the interface can be modified by the presence of the electrolytes. Vibrational spectra at these interfaces (IR, Raman and SFG) are calculated from the trajectories in order to relate structural properties to vibrational signatures, and make a direct link to experiments. Vibrational signatures are interpreted in relation with the microscopic structure of interfacial water molecules and electrolytes. The acido-basic characters of the quartz surface sites are also investigated once the aqueous surface is in contact with the electrolytes. Tentative conclusions relative to chemical reactivity & catalysis at these interfaces will be presented.

Some of the works presented here are done in collaboration with Prof M. Sulpizi (Johannes Gutenberg University, Mainz, Germany)

Just published: M. Pfeiffer-Laplaud, M.P. Gaigeot, J. Phys. Chem. C 2016, 120, 4866.

Tuesday, May 3, 09:45

## **Water orientation and hydrogen-bond structure at the fluorite/water interface**

Marialore Sulpizi

Johannes Gutenberg University Mainz, Staudinger Weg 7, 55099 Mainz/Germany

Water in contact with mineral interfaces is important for a variety of different processes. Here, we present a combined theoretical/experimental study which provides a quantitative, molecular-level understanding of the ubiquitous and important  $\text{CaF}_2$ /water interface. Our results show that, at low pH, the surface is positively charged, causing a substantial degree of water ordering. The surface charge originates primarily from the dissolution of fluoride ions, rather than from adsorption of protons to the surface. At high pH we observe the presence of Ca-OH species pointing into the water. These OH groups interact remarkably weakly with the surrounding water, and are responsible for the free OH signature in the Vibrational Sum Frequency Generation spectrum, which can be explained from local electronic structure effects. The quantification of the surface termination, near-surface ion distribution and water arrangement is enabled by a combination of advanced phase-resolved Vibrational Sum Frequency Generation spectra of  $\text{CaF}_2$ /water interfaces and state-of-the-art ab initio molecular dynamics simulations which include electronic structure effects.

Tuesday, May 3, 11:00

## Oxide stability and defect chemistry in an electrochemical environment: an ab initio perspective

Mira Todorova and Jörg Neugebauer

Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Most processes of practical importance constitute an inherently multidimensional problem, involving different length and time scales. Electrochemical processes, for example corrosion, present a particular challenge because of the involvement of the liquid phase. The prerequisite for developing strategies to counteract corrosion is understanding and quantitatively describing how materials behave in a corrosive environment. This requires not only information from the macroscopic scale down to the most fundamental level of electrons and atoms, but also involves very different materials classes with dissimilar characteristics, i.e. metals, semiconductors/insulators and liquid electrolytes. Point defects are a common attribute of each phase within a corroding system. They facilitate a seamless connection between quantum-mechanical calculations and environmental conditions impacting the corroding system, as well as between different phases of a corroding system via chemical potentials. This enabled us to develop an approach based on a fully grand-canonical description of both ions and electrons, that unifies and translates theoretical concepts from the fields of semiconductor defect chemistry and electrochemistry [1], and naturally links ab initio calculations to experimental observables, such as pH and  $U$  (the electrode potential). Employing this approach provides surprising new insight into apparently old problems like water stability, opens new routes to construct electrochemical phase (Pourbaix) diagrams, gives a handle on an absolute alignment of electrochemical potentials and provides insight into which point defects control the growth and dissolution of the oxide barrier layer formed when a metal comes into contact with a corrosive environment. Using the example of ZnO we employ the new approach to construct defect stability phase diagrams [2], which depict the dominant native point defects of band-gap materials, can be used to identify areas of interest in the context of electrochemical applications, and provide insight which impacts our understanding of fundamental corrosion mechanisms [3] and suggest routes to counteract corrosion.

[1] M. Todorova and J. Neugebauer, *Phys. Rev. Appl.* **1**, 014001 (2014).

[2] M. Todorova and J. Neugebauer, *Surf. Sci.* **631**, 190-195 (2015).

[3] M. Todorova and J. Neugebauer, *Farad. Discussions* **180**, 97-112 (2015).

Tuesday, May 3, 11:45

## **Coupling of Density-Functional Theory with Continuum Methods for Solid/Liquid Interfaces and Electrochemistry**

Richard G. Hennig

Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA

Solid-liquid interfaces are at the heart of many technologies ranging from catalysis to energy storage and conversion. We developed an implicit solvation method that describes the thermodynamically averaged interaction of the solute with the solvent and mobile ions for plane-wave density-functional theory and implemented it into the widely used plane-wave DFT code VASP. The latest VASPsol package (<http://vaspsol.mse.ufl.edu>) includes the description of dielectric and ionic screening using the Poisson-Boltzmann equation. We benchmark the method on solvation energies of small molecules and on the potential of zero charge of metal electrodes by comparing with experimental data and results using an explicit description of solvation. The solution of the Poisson-Boltzmann equation provides a unique reference for the electrostatic potential even in charged systems due to the shielding provided by the ions in the solution. This enables calculations of adsorption and reaction energies as function of applied electric potential. To demonstrate the utility of the implicit electrolyte model we apply the model to study the effect of electrolyte and external voltage on the adsorption energy of platinum atoms on a Pt(111) electrode. The results confirm experimental observations, that the Pt dissolution rate rapidly increases for externally applied potentials above 1 V. This illustrates the utility of the implicit VASPsol model for computational electrochemistry simulations.

Tuesday, May 3, 14:30

## **Operando synchrotron X-ray scattering studies of electrochemical interfaces**

Olaf M. Magnussen

Institute of Experimental and Applied Physics, Kiel University/Germany

Modern synchrotron sources provide X-ray radiation of high photon energy and extreme brilliance. These X-ray beams are powerful tools for the structural characterization of electrochemical interfaces, under non-equilibrium conditions and during interface reactions. In the talk examples and novel developments in the methodological capabilities of these techniques will be discussed, focusing on processes with relevance to electrocatalysis. Specifically, studies of the structural changes of metal electrodes during oxidation/reduction reactions on the atomic or nanometer scale will be presented for the case of Pt and Co. By detailed surface X-ray diffraction (SXR) studies and parallel single crystal voltammetry the place exchange between metal and oxygen atoms during Pt(111) oxidation was determined quantitatively, revealing a fully reversible surface restructuring up to a threshold coverage of exchanged Pt surface atoms. The temporal evolution of lateral mounds formed at higher potentials in oxidation/reduction cycles was measured by in situ grazing incidence small angle x-ray scattering (GISAXS) as a function of cycle number and potential, revealing a characteristic saturation behavior. SXR studies of Co oxides, motivated by recent interest in these materials as Pt-free catalysts for OER reaction, were performed on thin epitaxial Co(001) films, formed by electrodeposition on Au(111). Co hydroxide formation in alkaline solution is found to proceed via fast formation of an ultrathin passivating layer, followed by nucleation and growth of 3D hydroxide crystals at the grain boundaries in the Co deposit. Finally, first results by in situ transmission surface diffraction (TSD) at high photon energies are presented. This novel methods allow direct imaging of the entire in-plane structure of solid surfaces and ultrathin films in liquid environment and is capable of mapping structural properties on the micrometer scale.

Tuesday, May 3, 15:15

## Unravelling charging dynamics in subnanometre pores: an overview

Alexei A. Kornyshev

Department of Chemistry, Faculty of Natural Sciences, Imperial College London, SW7 2AZ, UK

Having smaller energy density than batteries, supercapacitors have exceptional power density and cyclability. Their energy density can be increased using ionic liquids and electrodes with subnanometre pores, but this tends to reduce their power density and compromise the key advantage of supercapacitors. To help address this issue through material optimization, we unravelled the mechanisms of charging subnanometre pores with ionic liquids, using molecular dynamics simulations, navigated by a phenomenological models.

Understanding dynamic properties is, however, impossible without understanding equilibria. I thus first overview the equilibrium properties and the various models that have been proposed to describe it (including the effect of anomalous capacitance, optimization of energy storage and other features), and then will proceed to dynamics.

In dynamics we have shown that charging of ionophilic pores is a diffusive process, often accompanied by overfilling followed by de-filling. In sharp contrast to conventional expectations, charging is fast because ion diffusion during charging can be an order of magnitude faster than in the bulk, and charging itself is accelerated by the onset of collective modes. Further acceleration can be achieved using ionophobic pores by eliminating overfilling/de-filling and thus leading to charging behaviour qualitatively different from that of in conventional, ionophilic pores. We have also studied the consequences of these effects in cyclic charging-discharging of the pores, characterised by CVs.

Similar kind of MD-simulations in cylindrical, quasi-single file pores are difficult to perform. We therefore derived for that case a continuum theory that in a number of aspects give results similar to our studies of the charging process in slit pores. In particular, it also predicts faster charging of ionophobic pores.

The revealed trends and dependencies await experimental verification. The overview is based on a series of works performed by an international team of authors listed in the literature review, and whose contributions will be highlighted in the talk.

### Literature

1. S.Kondrat and A. Kornyshev, Charging dynamics and optimization of nanoporous supercapacitors, *J. Phys. Chem. C* **117**, 12399-12406 (2013).
2. S.Kondrat, P.Wu, R. Qiao, A. A. Kornyshev, Accelerating charging dynamics in subnanometer pores, *Nature Mater.* **13**, 387-393(2014).
3. Y. He, J. Huang, B.G. Sumpter, A.A.Kornyshev, R.Qiao, Dynamic Charge Storage in Ionic Liquids-Filled Nanopores: Insight from a Computational Cyclic Voltammetry Study, *J. Phys. Chem. Lett.* **6**, 2230 (2015).
4. A. A. Lee, S. Kondrat, G. Oshanin, A. A. Kornyshev, Charging dynamics of a supercapacitor with narrow cylindrical Nanopores, *Nanotechnology* **25**, 315401, 1-8 (2014).
5. S. Kondrat and A.A.Kornyshev, Pressing a spring: what does it take to maximize the energy storage in nanoporous supercapacitors? , *Nanoscale Horizons*, **B1**, 45-52 (2016).
6. A.A.Kornyshev, The simplest model of charge storage in single file metallic nanopores, *Faraday Disc.* **164**, 117-133 (2013).
7. C.C. Rochester, G.Pruessner, and A.A.Kornyshev, Statistical mechanics of “unwanted electroactuation” in Nanoporous Supercapacitors, *Electrochim. Acta* **174**, 978-984 (2015).
8. G. Feng, X. Jiang, Rui Qiao, A. A. Kornyshev, Water in Ionic Liquids at Electrified Interfaces: The Anatomy of Electrosorption, *ACS Nano* **8**, 1168511694 (2014).
9. A.A.Lee, S. Kondrat, A.A. Kornyshev, Single-file charge storage in conducting nanopores, *Phys. Rev. Lett.* **113**, 048701, 1-5 (2014).
10. M.V.Fedorov and A.A.Kornyshev, Ionic liquids at electrified interfaces, *Chem. Rev.* **114**, 29783036 (2014).

Tuesday, May 3, 16:30

## **Ionic Liquids at Charged Surfaces and inside Nanoporous Electrodes**

Dmitry Bedrov and Jenel Vatamanu

Department of Materials Science & Engineering, University of Utah, Salt Lake City/USA

Electrical double layer capacitors (EDLCs), or supercapacitors, continue to gain an increasing attention as promising electrical energy storage devices that store energy via the accumulation of ions in a nanometer-thick layer at electrochemically-stable high specific surface area active electrodes. A notable improvement in EDLC performance has been achieved due to recent advances in understanding charge storage mechanisms, development of advanced nanostructured electrodes and electrochemically stable electrolytes such as room temperature ionic liquids. Despite extensive experimental work on these systems, the specifics of what happens inside and on the surfaces of nanostructured electrodes are still not well understood. In this presentation, I will discuss the results of our latest molecular dynamics simulations using state-of-the-art methodologies and focusing on gaining insight into understanding the molecular level phenomena that influence EDLC performance. Specifically, the presentation will focus on: a) the complex dependence of the capacitance on electrolyte double layer structure, electrode voltage and polarity, b) the influence of surface topography and nanopore dimensions/morphology on the charge storage mechanisms, and c) the issues associated with ion dynamics in charged nanostructures. The obtained molecular simulations results are discussed in light of reported experimental data and observations.

Tuesday, May 3, 17:15

## The reactivity of bimetallic electrodes at the atomic scale level: A challenge for the experimentalist

Sylvain Brimaud

Institute of Surface Chemistry and Catalysis Ulm University

The enhancement of the reaction rate for the electrocatalytic transformation of small molecules on metal electrode surfaces after addition of a second metal is well-known from numerous empirical investigations. Nowadays, computational chemistry provides a general framework which rationalizes the properties of bimetallic electrodes at the scale of the catalytic site: shifts of the metal d-band center are correlated with changes in the adsorbates binding energies [1, 2] and scaling relations between the binding energies of the reaction intermediates [3, 4]. The determination of a simple and unique descriptor, such as the DFT-computed binding energy of only one reaction intermediate for multi-step reactions, is believed to be predictive for the relative catalytic surface properties of bimetallic catalytic surfaces.

From the experimentalists perspective the accuracy of the measurements, the magnitude of the discrepancy between idealization and actual surface structure on which the investigations are conducted and, more specifically possible potential-induced restructuring of the electrode surface structure under reaction conditions are complex issues that have to be examined with great care. Since only a minor fraction of the surface catalytic sites may be responsible for the overall catalytic activity observed experimentally, the conclusion of structure / catalytic properties relationship for bimetallic electrodes at the atomic scale level from experimental results stays challenging and has to be carefully demonstrated.

Employing various well-defined bimetallic electrodes prepared either under ultra-high vacuum conditions [5-7], such as monolayer surface alloys or metal monolayers on heterometal substrate, or under electrochemical conditions [8], we will i) illustrate our current limit of accuracy for the experimental determination of the reactivity of bimetallic electrodes and ii) support with experimental results the relevance of these modern theoretical concepts for the rationalization of the relationship between the electrode surface structure and its electrocatalytic properties for the oxygen reduction reaction and the CO electrooxidation. We will also identify and discuss some factors playing important role in the reaction kinetics under realistic conditions which should not be underestimated in the establishment of a good agreement between experience and theory.

1. B. Hammer, J.K. Nørskov, *Adv. Catal.* **45** (2000) 71.
2. M. Mavrikakis, B. Hammer, J.K. Nørskov, *Phys. Rev. Lett.* **81** (1998) 2819.
3. F. Abild-Pedersen, J. Greeley, F. Studt, T.R. Munter, P.G. Moses, E. Skulason, T. Bligaard, J.K. Nørskov, *Phys. Rev. Lett.* **99** (2007) 016105.
4. J. Rossmeisl, A. Logadottir, J.K. Nørskov, *Chem. Phys.* **319** (2005) 178.
5. S. Brimaud, A.K. Engstfeld, O.B. Alves, H.E. Hoster, R.J. Behm, *Top. Catal.* **57** (2014) 222.
6. S. Brimaud, A.K. Engstfeld, O.B. Alves, R.J. Behm, *J. Electroanal. Chem.* **716** (2014) 71.
7. A.K. Engstfeld, S. Brimaud, R.J. Behm, *Angew. Chem. Int. Ed.* **53** (2014) 12936.
8. S. Brimaud, R.J. Behm, *J. Am. Chem. Soc.* **135** (2013) 11716.

Tuesday, May 3, 17:45

## Electrocatalysis on Stepped Surfaces

Fernanda Juarez<sup>1</sup>, Andres Ruderman<sup>1,2</sup>, Milagros Avila<sup>2</sup> and Elizabeth Santos<sup>1,2</sup>

<sup>1</sup> Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

<sup>2</sup> Facultad de Matemática, Astronomía y Física, Instituto de Física Enrique Gaviola (IFEG-CONICET),  
Universidad Nacional de Córdoba, 5000 Córdoba, Argentina

It is well known that defects play an important role in determining the properties of the electrodes. Systematic investigations of stepped surfaces, which allow a systematic control of the density of defects, are important tools to understand the mechanisms involved in electrochemical reactions of interest in electrocatalysis.

We have studied the hydrogen evolution reaction (HER) and metal decoration of stepped metal surfaces combining experiments and theory. On (111) silver surfaces, current transients were measured in order to obtain the kinetic constants of the HER. From a theoretical point of view, this reaction was also studied by combining Density Functional Theory (DFT), Molecular Dynamics (MD), Kinetic Monte Carlo (KMC), and our Electrocatalysis Theory. Adsorption energies of H were calculated on different sites, finding that the adsorption is stronger on the step than on the terraces. Activation barriers of the Volmer process were calculated for (100) and (111) surfaces. We found that the barrier is lower on the step, whereas on the terrace of the (111) it is larger than on the (100) flat surface.

Finally, we have investigated the metal decoration with Cu, Pt, and Pd of the (111) gold surface. Similarly to hydrogen on vicinal silver surfaces, the adsorption is stronger on the steps. However, there is a larger barrier to overcome the steps, in the case of the metals.

Wednesday, May 4, 09:00

## **Bifunctional ORR and OER Electrocatalysis for Metal-oxygen Batteries: Role of the Catalyst**

Christoph Bondu, Philipp Reinsberg, Hatem M. A. Amin, Lingxing Zan, Christoph Molls,  
Helmut Baltruschat

University of Bonn, Bonn/Germany

For metal air batteries, a highly reversible electrocatalyst is needed, i. e. a catalyst for both OER and ORR. In alkaline solution, Ag is known to be the best electrocatalyst for oxygen reduction. However, Ag is not catalyzing oxygen evolution. Spinels such as  $\text{Co}_3\text{O}_4$  and various Perovskites have been shown to be good catalysts for oxygen evolution but are not very good for oxygen reduction. We have recently shown that a particular mixture of a Ag catalyst with  $\text{Co}_3\text{O}_4$  nanoparticles leads to a catalyst which not only combines the good performance of Ag for the ORR with that of  $\text{Co}_3\text{O}_4$  for the OER, but shows a better activity than its components [1, 2].

Here, we will present further insights and demonstrate that this effect is also observed for various perovskites. The effect is also observed when  $\text{Co}_3\text{O}_4$  or the perovskites are deposited on smooth Ag electrodes. Using differential electrochemical mass spectrometry (DEMS) and  $^{18}\text{O}$  - isotope exchange has been shown in the past that during oxygen evolution at oxides the oxygen of the lattice is participating in the oxygen evolution reaction [3-4].

In aprotic solvents, oxygen reduction leads to superoxide or peroxide, depending on the cation present. Since no bond breaking is occurring here, a dependence of the reaction on the electrocatalyst material is not expected.

We have carried out a detailed study involving DEMS, electrochemical quartz crystal microbalance (EQCM) and the rotating disc electrode (RRDE) using a variety of smooth model electrodes (glassy carbon, different noble metals and Au(111)) and found marked differences. E.g., during oxygen reduction in a  $\text{Li}^+$  containing DMSO, reduction to superoxide and peroxide occur in well separated potential regions, whereas on Rh reduction occurs in a 2 electron process (as demonstrated by DEMS) in the whole reduction region. In the presence of Li, only a part of the formed reduction product ( $\text{Li}_2\text{O}_2$ ) is deposited on the electrode, another part is dissolved in the electrolyte. From the deposit, oxygen can be evolved, the amount of which also depends on the electrode material. Whereas on Pt and Rh the oxidation occurs in only one oxidation peak (which is paralleled by oxygen evolution) close to the equilibrium potential, on Au three peaks are observed in a wide potential range.

Comparative experiments using other electrolyte systems and in  $\text{Mg}^{2+}$  and other cation - containing electrolytes will also be presented.

Acknowledgement: Funding of this project by the BMBF (LuLi - project 03X4624A) and Mg - Luft, 03SF0447A) is gratefully acknowledged.

### References:

- [1] H.M.A. Amin, H. Baltruschat, D. Wittmaier and K.A. Friedrich, *Electrochim. Acta*, 151 (2015) 332.
- [2] D. Wittmaier, N. Wagner, K.A. Friedrich, H.M.A. Amin and H. Baltruschat, *J. of Power Sources*, 265 (2014) 299.
- [3] M. Wohlfahrt-Mehrens and J. Heitbaum, *Journal of Electroanal. Chem.*, 237 (1987) 251.
- [4] S. Fierro, T. Nagel, H. Baltruschat and C. Comninellis, *Electrochem. Com.*, 9 (2007) 1969.
- [5] C. J. Bondue, A. A. Abd-El-Latif, H. P. and H. Baltruschat, *J. Electrochemical Soc.* 162 (2015), A479-A487
- [6] C. J. Bondue, P. Reinsberg, A. A. Abd-El-Latif, H. Baltruschat, *Physical Chemistry Chemical Physics* 17 (2015), 25593

Wednesday, May 4, 09:30

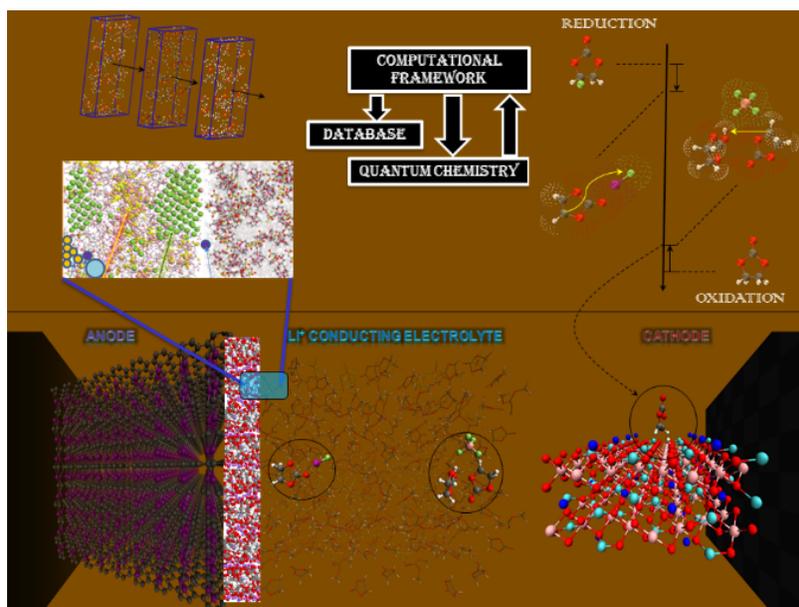
## Modelling Lithium Battery Electrolytes and Solid Electrolytes Interphases

Oleg Borodin

Electrochemistry Branch, Sensor and Electron Devices Directorate, U.S. Army Research Laboratory Adelphi, MD, 20783, USA

Tailoring electrolyte electrochemical properties is critical for stabilizing the electrode electrolyte interfaces and enabling novel electrochemical couples in lithium batteries. The rational design of an electrolyte requires not only the knowledge of the limits of electrolyte electrochemical stability and electrolyte decomposition reactions that might or might not occur at the surface of the electrode but also understanding of the structure and transport properties of the passivation film formed at the anode and/or cathode surfaces. I will discuss application of the molecular modelling methodologies to predict electrolyte electrochemical stability, decomposition reactions at electrodes, initial stages of the passivation layer formation and its properties.

When combined with accurate predictions of the electrolyte structure, such calculations provide tremendous insight into the mechanism of the in-situ formation of a highly beneficial passivation layer on electrodes that enable a wide range of electrode couples from lithium metal to conversion cathodes in non-aqueous electrolytes. Molecular modelling of the electrolyte structure and SEI formation mechanism enabling high energy density electrode couples in electrolytes will be discussed.



Wednesday, May 4, 11:00

## **Electrochemistry at Haldor Topsøe**

Søren Dahl

Haldor Topsøe A/S, Denmark

With the increasing electrification of society new business possibilities open up for a catalyst company like Haldor Topsøe. The talk will describe some of the work we do and have done on rechargeable batteries and high temperature electrolysis. Apart from a description of the technologies there will also be focus on the business reasons for us to work on them.

Wednesday, May 4, 11:45

**Molecular materials for electrochemical energy storage: From computational screening to adaptive QM/MM simulations**

Martin Korth

Institute of Theoretical Chemistry, Ulm University, Ulm/Germany

A status report is given on our work to combine empirical valence band (EVB) and adaptive QM/MM methods to model proton transfer through water to electrodes. We furthermore show how some of the developments made in this project into our overall strategy for the design of new molecular materials for electrochemical energy storage, based on fast computational screening, intermediate-level scans and detailed, adaptive QM/MM simulations, as well as close integration with subsequent experimental work.

# Poster titles

## **Electrocatalytic activity of structurally well defined $\text{Ag}_x\text{Pt}_{1-x}/\text{Pt}(111)$ monolayer surface alloys – correlation between structure and reactivity**

S. Beckord, S. Brimaud and R.J. Behm

Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

## **Theoretical elucidation of Pt(111) surface oxidation: from UHV to electrochemical conditions**

Donato Fantauzzi, Jonathan E. Mueller, and Timo Jacob

Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany, and

Institute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany

## **A theoretical study of single-walled gold nanotubes: atomistic origins of the capacitance of narrow tubes**

Aleksej Goduljan<sup>1</sup>, Fernanda Juarez<sup>1</sup> Elizabeth Santos<sup>1,2</sup>, and Wolfgang Schmickler<sup>1</sup>

<sup>1</sup> Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

<sup>2</sup> Facultad de Matemática, Astronomía y Física, Instituto de Física Enrique Gaviola (IFEG-CONICET), Universidad Nacional de Córdoba, 5000 Córdoba, Argentina

## **Electrocatalysis of Formate on Noble Metals**

J. Hermann, A. Abdelrahman, M. Al-Shakran, L.A. Kibler

Institute of Electrochemistry, Ulm University, 89069 Ulm, Germany

## **Diffusion properties of anode metals studied using DFT: growth phenomena and the effect of an electric field**

Markus Jäckle<sup>1,2</sup> and Axel Groß<sup>1,2</sup>

<sup>1</sup> Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, Helmholtzstr. 11, 89069 Ulm, Germany

<sup>2</sup> Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

## **Electro-oxidation of methanol on pseudomorphic grown Pt-multilayers on Ru(0001)**

J. Klein<sup>1</sup> F. Argast<sup>1</sup>, A.K. Engstfeld<sup>1,2</sup>, S. Brimaud<sup>1</sup> and R.J. Behm<sup>1</sup>

<sup>1</sup> Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

<sup>2</sup> DTU Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

## **Oxygen Evolution Reaction on MBE-grown $\text{SrIrO}_3$**

Jan Kloppenburg and Geoffroy Hautier

Institut de la matiere condensée et des nanosciences, Université catholique de Louvain,

B-1348 Louvain-la-Neuve, Belgium

**Structure, stability and local reactivity of metal surface alloys: a combined DFT and kMc study**

Luis Mancera and Axel Groß

Institute of Theoretical Chemistry, Ulm University, 89069 Ulm/Germany

**Electrochemical flow cell studies of oxygen reactions on Pd<sub>x</sub>Ag<sub>1-x</sub> bulk single crystals**

M.P. Mercer and H.E. Hoster

Lancaster University, Bailrigg, Lancaster, LA1 4YW, United Kingdom

**Intercalation of Alkali Halides in Carbon Nanotubes: A Theoretical Study**

Leila Mohammadzadeh<sup>1,2</sup>, Paola Quaino<sup>2</sup>, and Wolfgang Schmickler<sup>1</sup>

<sup>1</sup> Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

<sup>2</sup> PRELINE, Universidad Nacional del Litoral, Santa Fe, Argentina

**Dynamics of decay: investigations of the structural evolution of Pt<sub>2</sub>Ru catalysts during formate oxidation**

Jonathan E. Mueller<sup>1,2</sup>, Hana Hoffmannova<sup>3</sup>, Tetsuya Hiratoko<sup>3</sup>, Petr Krtil<sup>3</sup>, Timo Jacob<sup>1,2</sup>

<sup>1</sup> Institute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany

<sup>2</sup> Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany.

<sup>3</sup> J. Heyrovský Institute of Physical Chemistry, Dolejškova 3, Prague 18223, Czech Republic.

**Understanding interfacial water through 2D water polymorphs**

Tanglaw Roman and Axel Groß

Institute of Theoretical Chemistry, Ulm University, 89069 Ulm/Germany

**Accounting the electrochemical environment in the first principles calculation of electro-oxidation of methanol**

Sung Sakong and Axel Groß

Institute of Theoretical Chemistry, Ulm University, 89069 Ulm/Germany

**Water adsorbed on Pt layers grown pseudomorphous on Ru(0001) – a structural STM investigation on the vertical ligand effect**

M. Schilling, S. Brimaud and R.J. Behm

Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

**Preparation, Characterization and Electrocatalytic Activity of Bimetallic Pt<sub>x</sub>Ag<sub>y</sub> and Pd<sub>x</sub>Ag<sub>y</sub> Nanocrystals**

I. Weber, S. Brimaud<sup>1</sup>, J. Solla-Gullón<sup>2</sup>, J.M. Feliu<sup>2</sup> and R.J. Behm<sup>1</sup>

<sup>1</sup> Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

<sup>2</sup> Institute of Electrochemistry, University of Alicante, 03080 Alicante, Spain

## List of participants

	Name	Affiliation	Role
1	Al-Shakran, Mohammed	Ulm University	Poster Presenter
2	Baltruschat, Helmut	University of Bonn	Speaker
3	Beckord, Stephan	Ulm University	Poster Presenter
4	Bedrov, Dmitry	University of Utah	Speaker
5	Behm, R. Jürgen	Ulm University	PI FOR 1376
6	Borodin, Oleg	Army Research Laboratory	Speaker
7	Brimaud, Sylvain	Ulm University	Speaker
8	Chan, Karen	Stanford University	Speaker
9	Cucinotta, Clotilde	Trinity College Dublin	Speaker
10	Dahl, Søren	Haldor Topsøe A/S	Speaker
11	Dohm, Sebastian	Ulm University	Poster Presenter
12	Fantauzzi, Donato	Helmholtz Institute Ulm	Poster Presenter
13	Ferreira da Costa, Tamires	Ulm University	Poster Presenter
14	Gaigeot, Marie-Pierre	University of Evre	Speaker
15	Goduljan, Aleksej	Ulm University	Poster Presenter
16	Groß, Axel	Ulm University	Organizer, PI FOR 1376
17	Hennig, Richard	University of Florida	Speaker
18	Hermann, Johannes	Ulm University	Poster Presenter
19	Herrero, Enrique	University of Alicante	Speaker
20	Jäckle, Markus	Helmholtz Institute Ulm	Poster Presenter
21	Jacob, Timo	Ulm University	PI FOR 1376
22	Juarez, Fernanda	Ulm University	Speaker
23	Kibler, Ludwig	Ulm University	PI FOR 1376
24	Klein, Jens	Ulm University	Poster Presenter
25	Kloppenburger, Jan	University of Louvain	Poster Presenter
26	Kornychev, Alexei	Imperial College London	Speaker
27	Korth, Martin	Ulm University	Speaker
28	Magnussen, Olaf	University of Kiel	Speaker
29	Mahlberg, David	Ulm University	Poster Presenter
30	Mancera, Luis	Ulm University	Poster Presenter
31	Markovic, Nenad	Argonne National Lab	Speaker
32	Mercer, Michael	Lancaster University	Poster Presenter
33	Mohammadzadeh, Leila	Ulm University	Poster Presenter
34	Mueller, Jonathan	Ulm University	Poster Presenter
35	Nägele, Florian	Ulm University	Poster Presenter
36	Reuter, Karsten	Techn. Univ. of Munich	Speaker
37	Roman, Tanglaw	Ulm University	Poster Presenter
38	Rossmeisl, Jan	University of Copenhagen	Speaker
39	Sakong, Sung	Ulm University	Poster Presenter
40	Salmazo, Debora	Ulm University	Poster Presenter
41	Santos, Elizabeth	Ulm University	PI FOR 1376
42	Schilling, Martin	Ulm University	Poster Presenter
43	Schmickler, Wolfgang	Ulm University	PI FOR 1376
44	Spohr, Eckhard	Uni Duisburg-Essen	PI FOR 1376
45	Stephens, Ifan	DTU Lyngby	Speaker
46	Sulpizi, Marialore	University of Mainz	Speaker
47	Tillmetz, Werner	ZSW Ulm	Speaker
48	Todorova, Mira	MPI Düsseldorf	Speaker
49	Weber, Isabella	Ulm University	Poster Presenter
50	Yamagushi, Rodrigo	Ulm University	Poster Presenter
51	Zenonas, Jusys	Ulm University	PI FOR 1376

# Notes