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INVITATION

2ND INTERNATIONAL WORKSHOP:
SIMULATIONS OF/AT ELECTRODE INTERFACES

The AIT Austrian Institute of Technology and
CEST Centre of Electrochemical Surface Technology
invite you to the lecture series:

»SIMULATIONS OF/AT ELECTRODE INTERFACES«

Date Tuesday, 25th June 2013
Location CEST Centre of Electrochemical Surface Technology
Viktor-Kaplan-Straße 2, 2700 Wiener Neustadt

- 12.00** Arrival and Finger Food
- 13.00** **Christoph Kleber**, CEST, **Wolfgang Knoll**, AIT
Welcome
- 13.10** **Axel Groß**, University of Ulm:
"Challenges in the First-Principles Modeling of Electrochemical Electrode-
Electrolyte Interfaces"
- 13.50** **Alexander Auer**, MPI for Chemical Energy Conversion, Mülheim a. d. Ruhr:
"Modeling Electrochemistry - a Challenge for Quantum Chemistry"
Eckhard Spohr, University of Duisburg-Essen,
- 14.30** "Reactive Trajectory Approach to Proton Discharge from Aqueous
Solutions on Charged Metal Surfaces"
- 15.10** Coffee
- 16.00** **Timo Jakob**, University of Ulm:
„Understanding Electrochemical Interfaces“
- 16.40** **Stefan Freunberger**
"Fuel Cell Simulation on Various Relevant Length Scales"
- 17.20** **Notker Rösch**, Catalysis Research Center, TU Munich, and Institute of High
Performance Computing, Singapore:
"Nanostructured Mixed-Metal Systems"
- 18.00** End of lectures
- 18.30** Reception and 5 year anniversary celebration CEST

Date **Wednesday, 26th June 2013**
Location **CEST Centre of Electrochemical Surface Technology**
Viktor-Kaplan-Straße 2, 2700 Wiener Neustadt

- 9.00** **Omar Azzaroni**, University de la Plata, Argentina:
"Molecular Design of Electrode Surfaces Using Ionic Self-Assembly:
Applications in Biosensing and Bioelectrochemistry"
- 9.40** **Roland Ludwig**, BOKU Wien,
"Modeling and Simulation: Tools to Optimize the Performance of
Electrode-Bound Enzymes"
- 10.20** Coffee
- 10.40** **Julia Kunze**, TU Munich:
„Nanotubular TiOx/C Anodes for Lithium-Ion Intercalation“
- 11.20** **Lukas Andrejs**, AIT, Vienna,
„Evaluation of Surface Reactions at Anode Materials in LIB“
- 12.00** **Ulrich Stimming**, Physik Department E19 and Institute for Advanced
Study, TU Munich and TUM CREATE, Singapore: "The Importance of
Storage for Regenerative Electricity Production"
- 12.50** Concluding Remarks
- 13.00** End of Workshop

“Challenges in the First-Principles Modeling of Electrochemical Electrode-Electrolyte Interfaces”

Axel Groß

Institute of Theoretical Chemistry, Ulm University, and
Helmholtz Institute Ulm, D-89069 Ulm/Germany

In spite of its technological relevance in the energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces and electrical double layers is still rather limited. The theoretical description of these interfaces from first principles is hampered by three facts. i) In electrochemistry, structures and properties of the electrode-electrolyte interfaces are governed by the electrode potential which adds considerable complexity to the theoretical treatment since charged surfaces have to be considered. ii) The theoretical treatment of processes at solid-liquid interfaces includes a proper description of the liquid which requires to determine free energies instead of just total energies. This means that computationally expensive statistical averages have to be performed. iii) Electronic structure methods based on density functional theory (DFT) combine numerical efficiency with a satisfactory accuracy. However, there are severe shortcomings of the DFT description of liquids, in particular water, using current functionals.

Despite these obstacles, there has already significant progress been made in the first-principles modeling of electrochemical electrode-electrolyte interfaces. In this contribution, I will present our attempts [1-5] to contribute to this progress by systematically increasing the complexity of the considered systems. Thus we have addressed thermal disorder by performing ab initio molecular dynamics simulations [1], the DFT water description has been improved by including dispersion effects [2], varying electrode potentials have been considered in a numerical setup with an explicit counter electrode [3], water structures at stepped electrodes have been studied [4], and the fact that in equilibrium electrodes are typically covered by adsorbates has been taken into account [5].

[1] Schnur, S. and Groß, A. New J. Phys. 2009, 11, 125003.

[2] Tonigold, K. and Groß, A., J. Comput. Chem. 2012, 33, 695.

[3] Schnur, S. and Groß, A. Catal. Today 2011, 165, 129.

[3] Lin, X. and A. Groß, A., Surf. Sci. 2012, 606, 886.

[5] Roman, T. and Groß, A., Catal. Today 2013, 202, 1838.

CV Axel Groß

1993 Promotion „Vibrationsanregung zweiatomiger Moleküle bei Streuung an Oberflächen“ betreut von Prof. Dr. W. Brenig, durchgeführt am Physik-Department der Technischen Universität München

1993-1998 Wissenschaftlicher Angestellter in der Abteilung Theorie des Fritz-Haber-Instituts der Max-Planck-Gesellschaft in Berlin
Arbeitsgebiet: Dynamik der Molekül-Oberflächenwechselwirkung



- 1998-2004** C3-Professor für Theoretische Physik/Oberflächenphysik am Physik- Department der Technischen Universität München
- 1999** Habilitation Technische Universität Berlin „Ab initio Dynamikberechnungen von Reaktionen an Oberflächen“, Lehrbefähigung für das Fach Theoretische Physik
- 2004** C4-Professor und Leiter des Institutes für Theoretische Chemie an der Universität Ulm
- 2009-2012** Dekan der Fakultät für Naturwissenschaften
- 2012-** Sprecher des Fachverbandes Oberflächenphysik der Deutschen Physikalischen Gesellschaft
- 2012-2015** Vizepräsident für Forschung der Universität Ulm

"Modeling Electrochemistry - a Challenge for Quantum Chemistry"

Alexander Auer
 MPI for Chemical Energy Conversion, Mülheim a. d. Ruhr

In heterogenous and homogenous catalysis, quantum chemistry is a powerful tool to complement experimental techniques. In Electrochemical reactions, an additional component is present - the electrochemical potential. It not only influences the structure of the solvent in the vicinity of the reaction site, but also influences the electronic structure of the reactants and the interface. Modeling these reactions is a great challenge, and while in solid state physics many schemes exist, quantum chemical approaches have to be modified to develop their full potential. In this talk I will give an overview of advantages and disadvantages of quantum chemical methods in electrochemistry and show examples for applications and current developments in our group.

CV Alexander Auer

- 2011** Group leader (W2) in the department of Prof. F. Neese at the Max Planck Institute for Chemical Energy Conversion.
- 2010** Entitled "Honorarprofessor für computergestützte Quantenchemie" at the University of Technology, Chemnitz
- 2009** Group leader (W2) of the atomistic modelling group at the Max Planck Institute for Iron Research in the department of Prof. M. Stratmann, Düsseldorf.
- 2004** "Juniorprofessor für Theoretische Chemie" at the University of Technology, Chemnitz (positive evaluation 1.3.2007).
- 2002/2003** Postdoc in the group of Prof. M. Nooijen at Princeton University, funding by the NSF in the framework of the ITR (Information Technology Research) program.
- 2002** PhD thesis at the University of Mainz in theoretical chemistry in the group of Prof. J. Gauss "coupled cluster calculations of parameters of the nuclear magnetic resonance spectroscopy"



“Reactive Trajectory Approach to Proton Discharge from Aqueous Solutions on Charged Metal Surfaces”

Eckhard Spohr

Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, Essen, eckhard.spohr@uni-due.de

A reactive trajectory approach for the study of proton discharge from aqueous environments on charged metal surfaces is reviewed. It is based on an extension of a minimalistic empirical valence bond (EVB) model to study proton transfer in the bulk. Extensive quantum mechanical density functional theory calculations were parametrized for the EVB force field [1]. The model is used to investigate reactive (discharging) proton trajectories which were started in the bulk of a water film adsorbed on charged metal electrodes. The results indicate a transition between a reaction-dominated regime at moderate negative charges, where the rate constant increases exponentially, to a “transport limited” regime where the transfer rate is almost independent of the surface charge density (at highly negative surface charge densities) [2,3].

Recent extensions of the model and corresponding results of trajectory calculations to introduce background electrolytes with and without specific ion adsorption are presented. In NaCl solutions, e.g., it is found that the discharge rate is slowed down relative to that in pure water. We discuss how this phenomenon is associated with adsorption site-blocking by ions from the electrolyte, and with the reduced number of water pathways for Grotthuss style proton hops as a consequence of the presence of hydration shells containing water molecules in unfavourable arrangements for proton transfer.

[1] F. Wilhelm, W. Schmickler, R. R. Nazmutdinov, and E. Spohr, “A model for proton transfer to metal electrodes,” *J. Phys. Chem. C*, vol. 112, pp. 10814–10826, 2008.

[2] F. Wilhelm, W. Schmickler, and E. Spohr, “Proton transfer to charged platinum electrodes. A molecular dynamics trajectory study,” *J. Phys.: Condens. Matter*, vol. 22, p. 175001, 2010.

[3] F. Wilhelm, W. Schmickler, R. Nazmutdinov, and E. Spohr, “Modeling proton transfer to charged silver electrodes,” *Electrochim. Acta*, vol. 56, pp. 10632–10644, 2011.

CV Eckhard Spohr

Eckhard Spohr ist seit 1.7.2007 Professor für Theoretische Chemie am Campus Essen der Universität Duisburg-Essen. Seine im Bereich computational chemistry und computational material sciences beheimateten wissenschaftlichen Interessen liegen in der Strukturbildung und Dynamik von Molekülen und Verbänden in der kondensierten Phase. Hauptarbeitsgebiete sind die molekulare Computersimulation und Theorie von Elektrolytlösungen, sowie Transportprozesse an Grenzflächen und in porösen ungeordneten Materialien. Ein spezieller Schwerpunkt sind dabei Reaktivität und Transporteigenschaften von Materialien, die in der Brennstoffzellentechnologie Anwendung finden.



“Understanding Electrochemical Interfaces”

Timo Jacob

Institute of Electrochemistry, Ulm University, Ulm, Helmholtz Institute Ulm Electrochemical Energy Storage, Ulm, Karlsruhe Institute of Technology, Karlsruhe

The characterization of solid-liquid interfaces is of broad interest to electrochemistry since it is the place where electrochemical reactions occur. Several factors are influencing the nature of a given electrode/electrolyte interface such as the chosen metallic electrode, the solvent, the electrode potential, or the electrolyte. Also co-adsorbates from the electrolyte such as SO_4^{2-} , which might form ordered adlayers on metallic electrodes, affect the physicochemical processes, e.g. adsorption and desorption, metal deposition, corrosion, and the kinetics of electrochemical reactions. In this talk we will discuss how theoretical investigations that combine methods describing different length- and time-scales can be useful in determining the interfacial morphology and composition as well as ongoing electrocatalytic processes. In the first part, examples will be presented where *ab initio* studies combined with thermodynamic considerations helped in revealing the nature of the electrode under reaction conditions. Afterwards, electrode processes such as the electrochemical oxygen reduction reaction and the formic acid oxidation will be considered. Based on extensive first principles-based calculations on the reaction intermediates and transition states, we will discuss the ORR mechanism on Pt(111) electrodes [1]. After benchmarking our QM calculations to experimental data, we report a multi-pathway electrochemical ORR mechanism that is sensitive to reaction conditions, and specifically to the applied electrode potential. A simple analysis based on calculated rate constants remarkably reproduces experimentally known factors concerning the electrocatalytic ORR. Afterwards, we will use the thus-obtained QM information to deduce a reactive forcefield for larger scale molecular dynamics studies. Finally, I will discuss our recently formulated continuum approach to investigate an all-solid-state lithium-ion battery, consisting of transport equations and intercalation reactions [2]. Here the goal was to develop a bottom-up approach that is purely based on parameters and values computable from first principles. Besides comparing this formulation to “classical” approaches, possible model extensions are discussed.

[1] J. A. Keith, T. Jacob, *Angew. Chem. Int. Ed.*, 2010, 49, 9521.

[2] M. Landstorfer, T. Jacob, *Chem. Soc. Rev.*, 2013, DOI:10.1039/C2CS35050E

CV Timo Jacob

Timo Jacob studied physics at the University of Kassel, where in Feb. 2002 he received his PhD. After a two-years postdoctoral stay at Caltech, in 2004 he joined the theory department of the Fritz-Haber-Institute in Berlin, and finished his habilitation in theoretical physics at the Free University Berlin in Nov. 2008. In 2007 he became leader of an independent Emmy-Noether research group at the University of Ulm and received an ERC-StartingGrant in 2010. Since 2011 he is director of the institute of electrochemistry at Ulm University. His research interests are in multi-scale modeling of interfacial systems, including solid/gas- and solid/liquid-interfaces in electrochemical and non-electrochemical environments.



“Fuel Cell Simulation on Various Relevant Length Scales”

Stefan A. Freunberger

Institute for Chemistry and Technology of Materials, TU Graz

In polymer electrolyte fuel cells (PEFC) charge and mass transport and the intimately connected heat and current density distribution on all scales is of high interest for improving power density, which is associated to performance and costs. Despite considerable improvements, the major voltage losses in PEFCs arise from poor oxygen reduction kinetics, mass transport limitations and a high resistance of dehydrated ionomer. Catalyst activity and membrane conductivity are material specific properties. However, associated mass transport limitations and the hydration level of the ionomer are highly influenced by structural properties of the gas distributors. This is the morphology of the catalyst layer, mass transport properties of the micro porous layer (MPL) and the gas diffusion layer (GDL), and the flow field geometry. In terms of flow field geometry both the geometry of channels and ribs, the layout of the channels over the cell area, and the relative flow direction of the reactants come into play.

In this talk I will cover modeling efforts and associated experimental diagnostic of phenomena embracing all these length scales [1-7]. Both steady state and dynamic models are discussed.

[1] Freunberger, S. A., Reum, M., Evertz, J., Wokaun, A. & Buchi, F. N. Measuring the Current Distribution in PEFCs with Sub-Millimeter Resolution. *J. Electrochem. Soc.* 153, A2158-A2165 (2006).

[2] Freunberger, S. A., Santis, M., Schneider, I. A., Wokaun, A. & Buchi, F. N. In-Plane Effects in Large-Scale PEMFCs. *J. Electrochem. Soc.* 153, A396-A405 (2006).

[3] Freunberger, S. A., Wokaun, A. & Buchi, F. N. In-Plane Effects in Large-Scale PEFCs. *J. Electrochem. Soc.* 153, A909-A913 (2006).

[4] Schneider, I. A., Freunberger, S. A., Kramer, D., Wokaun, A. & Scherer, G. G. Oscillations in Gas Channels: Part I. The Forgotten Player in Impedance Spectroscopy in PEFCs. *J. Electrochem. Soc.* 154, B383-B388 (2007).

[5] Tehlar, D., Flueckiger, R., Wokaun, A. & Buechi, F. N. Investigation of Channel-to-Channel Cross Convection in Serpentine Flow Fields. *Fuel Cells* 10, 1040-1049 (2010).

[6] Zaglio, M., Schuler, G., Wokaun, A., Mantzaras, J. & Buechi, F. N. Parameter extraction from experimental PEFC data using an evolutionary optimization algorithm. *European Physical Journal-Applied Physics* 54 (2011).

[7] Zaglio, M., Wokaun, A., Mantzaras, J. & Buechi, F. N. 1D-Modelling and Experimental Study of the

CV Stefan Freunberger

Stefan Freunberger studied chemistry at Vienna University of Technology, Austria. For his master's and Ph.D. theses he moved to the Swiss Federal Institute of Technology (ETH) Zurich and the Paul Scherrer Institute, Switzerland to work on polymer electrolyte fuel cells. To investigate transport processes on a wide range of relevant scales he developed advanced models and novel experimental techniques. For postdoctoral work he joined the group of Prof. Peter G. Bruce FRS at the University of St. Andrews, Scotland, to work on fundamental aspects of the non-aqueous Li-O₂ battery.



For this work he earned a EPSRC early career fellowship. His contributions to this rapidly evolving field embrace the development of in-situ spectroscopic techniques, elucidation of the reaction mechanism, electrocatalysis and the important role of electrolyte and electrode substrate. He is author of over 30 peer reviewed publications, including in Science and Nature Materials. In 2012 Freunberger moved to ICTM at Graz University of Technology to build his own research within the lab of Prof. Martin Wilkening. His research focuses on electrochemical energy storage materials, electrolytes and reaction mechanisms for advanced non-aqueous battery chemistries and their ageing behavior.

“Nanostructured Mixed-Metal Systems”

Notker Rösch

Catalysis Research Center, TU München, and Institute of High Performance Computing Singapore

We will discuss DFT results for metal nanoislands adsorbed on metal surfaces, in particular the scaling of their properties. On the example of Pt nanoislands on Au and Cu surfaces, we will compare these nanostructured mixed-metal systems to the corresponding pseudomorphic overlayers. In addition, we will discuss progress and problems when modeling nanoalloy particles of several thousand atoms via a DFT approach.

CV Notker Rösch

After reading physics and mathematics at TU München, Notker Rösch completed his doctorate there with research on transport theory of chemical reactions. As postdoc in the US, at MIT and Cornell University, he turned to quantum chemistry, applying in particular density functional methods. Since 1980 he has been a professor of theoretical chemistry at TUM where he currently serves as Academic Director of the Catalysis Research Center. Since 2012 he also heads the newly founded Catalysis Modeling Group at the Institute of High-Performance Computing in Singapore. He has co-authored over 450 research papers and book chapters dealing with metal clusters and problems in relativistic density functional theory, surface science, biophysical chemistry, as well as homogeneous and heterogeneous catalysis.



“Molecular Design of Electrode Surfaces Using Ionic Self-Assembly: Applications in Biosensing and Bioelectrochemistry”

Omar Azzaroni

Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA) Universidad Nacional de La Plata – CONICET, azzaroni@inifta.unlp.edu.ar

Utilization of weak intermolecular forces for the construction of new supramolecular architectures with controlled dimensionality and their implementation in practical applications is a major theme in contemporary chemistry, nanoscience and materials science. Within this framework the concept of ionic self-assembly (ISA) holds unparalleled versatility for the facile creation of supramolecular materials. ISA exploits the functional capabilities of ionic surfactants and oppositely charged polyelectrolytes to form supramolecular mesostructures exhibiting excellent stability and stiffness. As a result this approach has found incredible resonance in the emerging field of “nanoarchitectonics” provided that it offers new strategies for the bottom-up assembly of integrated supramolecular systems displaying concerted functions. Current research on ISA has reached the frontiers of electrochemistry and consequently new electroactive ionically self assembled materials came to light.

In this context, the integration of biorecognizable units into the electroactive supramolecular material is of critical importance to further broaden the reach of ISA into the arena of bioelectrochemistry. This is particularly important if we consider that the combination of the ISA technique and redox glycoproteins with electrochemistry may offer new perspectives in the design of amperometric biosensors or biofuel cells. Successful immobilization and electrical contacting of redox proteins with conducting substrates constitute the cornerstone of modern bioelectrochemistry and represent critical events in the construction of bioelectrodes. Within this framework, recognition-directed biosupramolecular assembly emerged as an interesting and attractive alternative due to its simplicity and versatility, without introducing chemical modifications into the enzyme. In this presentation I will describe recent experiments illustrating the powerful combination of ionic self-assembly and recognition-directed assembly to immobilize and “wire” redox glycoenzymes on electrode supports using electroactive glycopolyelectrolytes as functional building blocks. Results reveal the potential of ISA to further broaden the range of possibilities to design “soft” heterosupramolecular films compatible with the integration of bioactive elements on electrode surfaces.

CV Omar Azzaroni

Omar Azzaroni studied chemistry at the Universidad Nacional de La Plata (UNLP) (Argentina), receiving his Ph.D. in 2004 for research involving the use of self-assembled monolayers in alternative nanofabrication techniques. His postdoctoral studies were carried out at the University of Cambridge (UK) (2004–2006, Marie Curie Research Fellow) and the Max Planck Institute for Polymer Research (Germany) (2007, Alexander von Humboldt Research Fellow). In 2008, he moved back to Argentina as a staff scientist of CONICET and established the Soft Matter Laboratory of the Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA).



He is currently holds the position of Vice-Director of INIFTA and Adjunct Professor of Physical Chemistry at UNLP. His research interests include new applications of polymer brushes, biorecognition-driven assembly on surfaces, nanostructured hybrid interfaces, supramolecular materials science.

“Modeling and simulation: tools to optimize the performance of electrode-bound enzymes”

Roland Ludwig

Department of Food Science and Technology, Vienna Institute of Biotechnology, BOKU – University of Natural Resources and Life Sciences, Vienna

The development of miniature enzymatic biosensors and biofuel cells aims at self-sustained, implantable, minimally invasive medical devices, which can gather spatially and temporally resolved chemical information in tissues or organs. Miniaturization, stability and accuracy are the targeted key features of these analytical biodevices. The basis of such enzymatic biosensors and biofuel cells is an efficient electron transfer between the bioelement and the electrode to obtain sufficient current output at maximum miniaturization. Direct electron transfer (DET) between bioelement and electrode is based on electron tunneling over short distances (<1.5 nm). Although DET it is observed for only a few enzymes it is an elegant approach to connect enzymes and electrodes without the need for redox mediators. Our research to develop a glucose/oxygen based biofuel cell was based on two enzymes capable of DET, namely cellobiose dehydrogenase as anode biocatalyst and laccase as cathode biocatalyst. To achieve maximum power output enzyme engineering was used to improve the catalytic activity, binding and orientation of both enzymes. Modeling tools and simulation techniques such as comparative modeling, substrate docking and molecular dynamics were used to optimize biocatalyst structure and performance in terms of substrate specificity, substrate turnover, resistance to inhibitors, orientation and electron transfer to the electrode surface.

CV Roland Ludwig

Born 1973 in Vienna, Roland Ludwig received his PhD in biochemistry from BOKU - University of Natural Resources and Applied Life Sciences, Vienna in 2004. He worked for five years as project manager and researcher on the development of industrial biocatalytic processes at the Austrian Centre of Industrial Biotechnology. In 2009, he was awarded an APART fellowship of the Austrian Academy of Sciences to study electron transfer reactions of redox enzymes on electrode surfaces at Lund University. He joined BOKU in 2011 again and is currently leading a research group focused on biocatalysis and bioanalytics and lecturing on related subjects.



“Nanotubular TiO_x/C anodes for lithium-ion intercalation”

Jassen Brumbarov, Vivek Padmanabhan, Silvia Leonardi and Julia Kunze
Physics Department E19 and Institute for Advanced Study (IAS),
Technische Universität Munich, Garching, Germany

Li intercalation experiments were conducted with TiO_x/C nanotubes [1] annealed in acetylene (C₂H₂) and argon (Ar) at 400°C to partially reduce the TiO₂ to TiO_x and to stabilize the reduced structure with carbon. Anatase TiO_x nanotubes annealed in Ar were used as a reference. The nanotubes have a diameter of 100 nm and a length of 700 nm. The intercalation of lithium (Li) in the TiO_x/C tubes appears at more positive potentials compared to the one for TiO_x nanotubes. The reversible capacity of anatase TiO_x/C at a low rate of 0.3 C (50 mA/g) is as high as 320 mAh/g, which is far above the theoretical value where Li_{0.5}TiO₂ (168 mAh/g) is formed as the Li-rich phase [2], whereas that of anatase TiO_x amounts to 141 mAh/g only. At a high rate of 6.0 C (1 A/g), still capacities of 155 mAh/g are observed for TiO_x/C, which demonstrates the high rate capability of the material

Composite electrodes of conductive titania nanotubes coated with silicon (Si) via chemical vapor deposition (CVD) were produced and studied in terms of their Li intercalation characteristics. Both components show Li-intercalation capacities close to their theoretical values of 168 mAh/g (Li_{0.5}TiO₂) and 4200 mAh/g (Li₂₂Si₅) [3] resulting in 340 mAh/g capacity for the composite containing 4.7wt.% Si. High capacity retention upon cycling was achieved owing to the good adhesion of the thin Si coating and the formation of a stable solid electrolyte interface (SEI) in ethylene-carbonate (EC), dimethyl-carbonate (DMC), vinylene-carbonate (VC) electrolyte with 1M LiPF₆.

[1] R. Hahn, F. Schmidt-Stein, J. Salonen, S. Thiemann, Y. Song, J. Kunze, V.-P. Lehto, P. Schmuki, *Angew. Chem. Int. ed.* 48 (2009) 7236.

[2] D. Bresser, E. Paillard, E. Binetti, S. Krueger, M. Striccoli, M. Winter, S. Passerini, *J. Power Sources* 206 (2012) 301.

[3] W.J. Weydanz, M. Wohlfahrt-Mehrens, R.A. Huggins, *J. Power Sources* 81 (1999) 237.

CV Julia Kunze

2012 Venia Legendi in Physical Chemistry, TUM, Chemistry & Physics Department.

2009-2012 Habilitation and Fellow of the TUM Institute for Advanced Study (IAS) with Prof. U. Stimming: Molecular Aspects in Interfacial Science – fundamentals and applications of materials for energy conversion and electrocatalysis in the context of nanoscience.

2004-2009 Senior Scientist at the Friedrich-Alexander Universität Erlangen-Nürnberg, Department of Materials Science and Engineering with Prof. P. Schmuki: Growth mechanisms and organic functionalization of oxide films.

2003-2004 Postdoctoral fellow at the University of Guelph, Department of Chemistry and Biochemistry with Prof. J. Lipkowski: In Situ Studies of the Structure and Optical Properties of Ordered Molecular Films and Biomimetic Membranes at Electrified Interfaces.

2002-2003 Postdoctoral fellow at the Heinrich Heine Universität Düsseldorf, Institut für Physikalische Chemie und Elektrochemie with



“Evaluation of Surface Reactions at Anode Materials in LIB”

Lukas Andrejs and Atanaska Trifonova
AIT Austrian Institute of Technology, Vienna

Rechargeable lithium ion cells operate at up to 4.2 V cell voltage. This is well beyond the thermodynamic stability window of the commonly used aprotic organic electrolytes. Hence, when the electrode is polarized to sufficient low potentials, the reductive electrolyte decomposition in parallel to irreversible consumption of lithium ions takes place at the electrode / electrolyte interface. The decomposition products build up a layer that covers the electrodes surface (Solid Electrolyte Interface-SEI). Today, it is widely accepted that a proper SEI is of utmost importance for good electrode functioning and thus for good battery performance. Important battery characteristics e. g., power fade, self-discharge, shelf life, cycle life, safety etc., strongly depend on the properties of the SEI layer. Therefore, investigations concerning SEI formation mechanisms are a key issue for Li-ion battery technology. In situ methods that allow monitoring changes deriving from electrolyte decomposition reactions in parallel to electrochemical measurements are outstanding tools in order to achieve a better understanding of the respective electrolyte decomposition mechanisms. Special emphasis is laid on the investigation of electrolyte reduction mechanisms at various Li-ion battery anode materials. (i.e., graphitic- and non-graphitic carbons, Li-storage alloys). Moreover, the SEI formation at low and high temperatures in different electrolyte systems will be presented.

CV Lukas Andrejs

Lukas Andrejs joined Austrian Institute of Technology's battery materials research team in January 2013. He studied at the Vienna University of Technology (TU Vienna), where he concentrated on chemistry and technology of materials. His diploma thesis was carried out in close cooperation with TDK-EPC Deutschlandsberg (former EPCOS OHG) while he also attended a parallel study programme at the Graz University of Technology at the same time. His dissertation, which he completed at the Christian Doppler Laboratory for Ferroic Materials at TU Vienna in 2009-2012, is in the area of solid state electrochemistry and defect chemistry, and focuses on resistance degradation and charge transport in lead zirconate titanate – a perovskite-type electroceramic material.



“The Importance of Storage for Regenerative Electricity Production”

Ulrich Stimming

Physik Department E19, Institute for Advanced Study, TU Munich, Garching, Germany, TUM CREATE, Singapore

It is an important goal to gradually substitute energy conversion based on fossil fuels by one based on regenerative energy sources. As a consequence, electricity production moves from a centralized (one producer and many consumers) to a decentralized (many producers and many consumers) operation. Thus, a completely revised architecture of energy systems seems necessary. Such novel architectures need to be supported by technical possibilities, a central one of them being that there are suitable electricity storage devices. While the efficiency is largely determined by the structure (=architecture) of energy systems, challenges lie in the performance of energy storage devices. Criteria are volumetric and gravimetric energy and power density, depending on the specific application, and costs. There are different technical approaches such as storage in batteries (in encased chemical energy), in super-capacitors (in charge in physical systems), or in chemicals (in hydrogen or others) for long term storage, the latter requires a converter (e.g. a fuel cell) to produce electricity. For stationary systems also physical systems such as compressed air or pumped hydroelectricity are possibilities worth considering (both also require a converter back to electricity). An important parameter is the time for which storage should be accomplished and how much self-discharge occurs. Technology needs to be evaluated under the aspect of centralized versus de-centralized energy systems. In a preliminary form, these are the two limiting cases for future energy systems where local electricity production and consumption decide which mixture of both is sensible and gives the largest benefit to producers and consumers of electricity.

CV Ulrich Stimming

Professor Ulrich Stimming is currently Scientific Advisor and Principal Investigator in TUM CREATE, a Research project on electromobility of the Technical University Munich (TUM) in Singapore; until the end of 2012 he was also the Chief Executive Officer of TUM CREATE. He is a Fellow of the Institute of Advanced Study of TUM. He was a Professor of Physics, chair E19, Interfaces and Energy Conversion, and of Chemistry at the Technical University of Munich, Germany and member of the Board of directors of the Bavarian Center of Applied Energy Research, ZAE Bayern. He has received his Ph.D. in Physical Chemistry from the Free University of Berlin; previously, he has held faculty positions at Columbia University in New York, U.S.A. and at the University of Bonn, Germany. He was also a director at the Research Center of Jülich where he set up a broad range fuel cell research program. Prof. Stimming is Editor-in-chief of the journal “Fuel Cells—from Fundamentals to Systems” published by Wiley-VCH. He received several international awards for his accomplishments. Currently, he is holding Visiting Professorships at the University of Yamanashi, Japan, Nanyang Technological University, Singapore and Shanghai Jiao Tong University, Shanghai, China.

