AKE 5: Mobilität

Time: Monday 16:45–18:15 Location: MENSA Dül

Invited Talk AKE 5.1 Mon 16:45 MENSA Dül

Energiespeicher für Elektromobilität Stand der Technik und Perspektiven — •Margret Wohlfahrt-Mehrens — ZSW Ulm

Die Entwicklung leistungsstarker und zuverlässiger elektrochemischer Energiespeichersysteme ist eine Schlüsseltechnologie für die Elektromobilität. Lithium-Ionen-Batterien sind derzeit die aussichtsreichsten Kandidaten für alternative Fahrzeugkonzepte. Sie weisen deutlich höhere Energie- und Leistungdichten als andere heute verfügbare Technologien wie Blei- oder Nickel/Metallhydridakkumulatoren auf. Energiedichte, Leistung, Lebensdauer und Sicherheit von Lithium-Ionen-Batterien werden wesentlich durch die Wahl der Aktivmaterialien und das Elektrodendesign bestimmt. Eine Vielzahl alternativer Elektrodenmaterialien befindet sich in der Entwicklung, um die Fahrzeuganforderungen besser erfüllen zu können. Dabei sind die Erforschung neuer Elektrolytsysteme und die Erarbeitung eines umfassenden Verständnisses der Grenzfläche Elektrode/Elektrolyt ebenfalls wichtige Voraussetzungen für die effiziente Weiterentwicklung langlebiger Hochenergiespeichersysteme. Der Vortrag gibt einen Überblick über die Anforderungen an automobile Speichersysteme, den Stand der Technik derzeit verfügbarer Speichertechnologien und die Anforderungen an Forschung und Entwicklung für zukünftige Hochenergie-Batterie-Generationen.

AKE 5.2 Mon 17:15 MENSA Dül

First-principle study and modeling of pressure dependent ionic diffusion in YSZ — •Julian Hirschfeld and Hans Lustfeld — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Yttria Stabilized Zirconia (YSZ) is the state of the art electrolyte for Solid State Fuel Cells (SOFC). YSZ has a low thermal expansion coefficient and good ionic conductivity at a high operation temperature (800°C). Since this temperature also dictates the operating point of the SOFC, it has to be reduced to achieve an economic operation of a SOFC. The temperature dependence of the ionic conductivity is given by an Arrhenius expression [1]. Due to the inverse exponential dependence on the activation energy, it is crucial to gain a better knowledge about the dependence of this quantity on external parameters. It is possible to obtain the activation energy of individual ionic jump processes directly from ab-initio calculations [2]. This can increase the fundamental understanding of the physics behind and can lead to predictions of new systems.

In our work we use Density Functional Theory (DFT) ab-initio calculations to investigate the ionic energy barrier dependence on structural deformations. To obtain the activation energies, we calculate the energy barrier of the ionic movement in the framework of the Nudged Elastic Band (NEB) method. To gain a deeper insight into the physical meaning, we compare these results with those of a simple model.

[1] M. Kilo et al., Phys. Chem. Chem. Phys. 5, 2219-2224 (2003)
[2] Pornprasertsuk et al., J. Appl. Phys. 98, 103513 (2005)

AKE 5.3 Mon 17:30 MENSA Dül

New double-cation borohydrides — •Inge Lindemann[1], Roger Domènech Ferrer[1], Yaroslav Filinchuk[2], Hans Hagemann[3], Radovan Černý[3], Ludwig Schultz[1], and Oliver Gutfleisch[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270016, 01171 Dresden, Germany — [2]Swiss-Norwegian Beam Lines at ESRF, BP-220, 38043 Grenoble, France — [3]Department of Physical Chemistry and Crystallography, University of Geneva, 1211 Geneva, Switzerland

Complex hydrides are under consideration for on-board hydrogen storage due to their high hydrogen density. However, up to now conventional borohydrides are either too stable or unstable for applications as in PEM fuel cells (60-120°C). Recently, double-cation borohydride systems have attracted great interest. The desorption temperature of the borohydrides decreases with increasing electronegativity of the cation. Consequentely, it is possible to tailor a feasible on-board hydrogen storage material by the combination of appropriate cations. The stability was found to be intermediate between the single-cation borohydride systems. Two combinations were sucessfully synthesised by metathesis reaction via high energy ball milling. Al-Li-borohydride shows desorption at about 70°C combined with a very high hydrogen density (17.2 wt.%) and the Na-Al-borohydride (14.2 wt.%) decomposes around 90°C. Both desorption temperatures are in the target range for applications. The decomposition pathways were observed by in-situ-Raman spectroscopy, DSC (Differential Scanning Calorimetry), TG (Thermogravimetry) and thermal desorption measurements.

Invited Talk AKE 5.4 Mon 17:45 MENSA Dül

Production and conversion of liquid fuels and hydrogen from biomass and natural gas using micro-reactor technology — •Peter Pfeifer — Karlsruhe Institute of Technology (KIT), Institute for Micro Process Engineering (IMVT), Herrmann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, www.imvt.kit.edu

The Institute for Micro Process Engineering (IMVT) develops microstructured devices since 1989 and is thus one of the pioneers in this field. One focus of current research is on the integration of catalysts into these reactors as this is significantly influencing the overall system performance. The methods are ranging from filling micro-structured elements with catalyst powder to new approaches of nano-structured catalyst layers on the micro channel walls. Current projects are addressing the field of conversion of synthesis gas from biomass feedstock and off-shore natural gas; processes are methanol synthesis, direct dimethyl ether synthesis, Fischer-Tropsch synthesis and high temperature / high pressure shift reaction. The latter reaction may be necessary for the biomass conversion into fuels since dry gasification yields an insufficient H2/CO ratio in the synthesis gas. The unusual temperature and pressure conditions applied in the IMVT concept reduce the net energy loss. Furthermore, most micro-reactor studies in literature refer to keeping the reaction temperature constant and thus enabling isothermal operation conditions. However, for synthesis, i.e. exothermic equilibrium reactions, a falling temperature profile should be applied. Heat management concepts for micro-reactors are therefore important for further developments.