

MM 42: Functional Materials I

Time: Thursday 17:45–19:00

Location: IFW B

MM 42.1 Thu 17:45 IFW B

Correlation of structural properties and electrochemical characteristics of carbon aerogel electrodes — ●VOLKER LORRMANN¹, GUDRUN REICHENAUER¹, VLADIMIR DYAKONOV^{1,2}, and JENS PFLAUM^{1,2} — ¹Bavarian Center of Applied Energy Research e.V. (ZAE Bayern), 97074 Würzburg — ²Experimental Physics VI, Julius-Maximilians-University of Würzburg, 97074 Würzburg

In electrochemical double-layer capacitors (EDLC) the energy is stored in the electrochemical double-layer interface between the electrode surface and the electrolyte solution. The capacitance of EDLCs and rate capability depend on the porous nanostructure of the electrodes. Carbon aerogels, based on sol-gel derived organic precursors, are promising candidates for EDLC electrodes because of their tunable nanostructure (e.g. pore- and particle size). For the same reason these materials also represent excellent model systems for the investigation of correlations between structural properties and electrochemical characteristics. We prepared carbon aerogel EDLC electrodes with different primary particle sizes using different catalyst concentration in the starting solution. Scanning electron microscopy measurements of the carbons show, that the particle size and hence the interparticular pores are varied between several ten nm up to some μm . Electrochemical investigation was performed by cyclic voltammetry and impedance spectroscopy in different electrolyte solutions. The relationship between the nanostructure and the electrochemical performance of the carbon aerogel is discussed.

MM 42.2 Thu 18:00 IFW B

Structure of layered covalent organic frameworks — ●BINIT LUKOSE, AGNIESZKA KUC, and THOMAS HEINE — School of Engineering and Science, Jacobs University Bremen, Bremen, Germany

Covalent-Organic Frameworks (COFs)[1] are a new family of 2D and 3D highly porous and crystalline materials built of light elements, such as boron, oxygen and carbon. For all 2D COFs, AA stacking arrangement has been reported on the basis of experimental powder XRD patterns, with the exception of COF-1 (AB stacking). The AA stacking arrangement maximizes the attractive London dispersion interaction between the layers, which is the dominating term of the stacking energy. At the same time, AA stacking always results in a repulsive Coulomb force between the layers due to the polarized connectors. In this work[2,3], we show that a set of reported and hypothetical 2D COFs are considerably more stable if their stacking arrangement is either serrated or inclined, and layers are shifted with respect to each other by $\sim 1.4 \text{ \AA}$. These structures are in agreement with to date experimental data, including the XRD patterns, and lead to a larger surface area and stronger polarization of the pore surface.

[1] Porous, crystalline, covalent organic frameworks. A. P. Cote, O. M. Yaghi, et al Science 310 (2005) 1166-1170

[2] Structure of layered covalent organic frameworks. B. Lukose, A. Kuc, T. Heine, Chem. Eur. J. (2010) accepted for publication.

[3] On the reticular construction concept of covalent organic frameworks. B. Lukose, A. Kuc, J. Frenzel, T. Heine, Beilstein J. Nanotechnol. 1 (2010) 60-70.

MM 42.3 Thu 18:15 IFW B

Study of the degradation of conjugated polymers using scanning probe microscopy — ●ESHA SENGUPTA, ANNA L. DOMANSKI, STEFAN A.L. WEBER, MARIA B. RETSCHKE, HANS JÜRGEN BUTT, and RÜDIGER BERGER — Max Planck Institute for Polymer Research, Mainz, Germany

A major problem for applications of conjugated polymers in organic photovoltaics is their limited life-time [1]. Degradation occurs when these are exposed to sunlight, oxygen and water. Recent studies have reported changes in the open circuit voltage (Voc) and short circuit

current (Jsc) in fabricated organic solar cells as estimates of degradation [2]. However, in these studies, device fabrication and optimization of the processing steps are time consuming. Since the morphology of organic solar cells needs to be controlled on a nanometer scale due to small exciton pathways, Scanning Probe Microscopy (SPM) provides a valuable tool to study topographic and electronic effects. Here, we present an SPM based method to study degradation of conjugated polymers without the need to fabricate devices. Changes in the surface potential and conductivity due to degradation of the active layer of solar cells were investigated using Kelvin Potential Microscopy (KPM) and conductive Scanning Force Microscopy (c-SFM). These changes have been related to the Voc and Jsc changes upon degradation. We expose the active layer directly to simulated sunlight and varying amounts of oxygen and humidity while partially covering it with a grid. [1] Krebs, F.C. et al., Chemistry of Materials, 2005, 17, 5235 [2] Seemann, A., et al., Organic Electronics, 2009, 10, 1424.

MM 42.4 Thu 18:30 IFW B

Hydrogen absorption behavior of nano-crystalline Mg thin films — ●HELMUT TAKAHIRO UCHIDA, REINER KIRCHHEIM, and ASTRID PUNDT — Institut fuer Materialphysik, Universitaet Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

In-situ XRD measurements of hydrogen absorption behavior were done for nano-crystalline Mg thin films at room temperature. 20 nm Pd-capped nanocrystalline Mg films of different thicknesses were prepared in an UHV chamber, by means of ion beam sputter deposition under Ar-atmosphere at the pressure of $2.2 \cdot 10^{-4}$ mbar. The Mg films were deposited on Si (100) substrates. XRD measurements using a Phillips X-Pert diffractometer with Co-K alpha radiation were performed before and after hydrogenation in order to check the phase transition and the change of the sample texture. In-situ XRD measurements have been done at the HASYLAB synchrotron facility in Hamburg and at European Synchrotron Facility in Grenoble. Changes of the resistivity during hydrogenation were also monitored by four-point measurement, during electrochemical- and gas pressure hydrogen loading. The diffusion coefficient of hydrogen in nano-crystalline Mg thin films at room temperature is estimated from in-situ synchrotron XRD measurements and compared with the results of electrochemical hydrogen permeation measurements. The impact of grain boundaries on the hydrogenation properties is discussed. Financial support by the DAAD, HASYLAB and the ESRF is gratefully acknowledged.

MM 42.5 Thu 18:45 IFW B

Investigation of Lithium diffusion in sputtered layers of lithium titanat — ●FABIAN WUNDE and GUIDO SCHMITZ — Institut für Materialphysik, WWU Münster, Deutschland

Lithium titanate (LTO) is used as an anode material for lithium ion batteries, as it reveals both, electronic as well as Li-ion conductivity. To investigate its ionic properties, ion-beam sputter-deposited thin films of LTO have been analysed by means of galvanostatic charge-discharge measurements. It has been observed that the measured charge capacities show a strong dependence on the charge/discharge current densities, i.e the charge capacity decreases when increasing the current. In order to explain this decrease in capacity, the kinetics of Li insertion into the LTO films is described by diffusion. Solving Fick's diffusion law with finite diffusion space while assuming a constant electrical current as boundary condition, leads to theoretical concentration profiles. Subsequent combination of these profiles with the well-known Nernst equation shows that the observed loss of capacity is due to a gradient of the Li concentration and therefore depends on the diffusion coefficient of Li in LTO. By evaluating the measured capacity loss as a function of current the diffusion coefficient is determined.