HL 12: Energy materials: Water splitting, batteries, and supercapacitors (with CPP/MM)

Time: Monday 10:45–12:30 Location: POT 081

HL 12.1 Mon 10:45 POT 081

Highly efficient photocatalytic water splitting with colloidal CdS nanorods by mediated hole scavenging — •Thomas Simon, Aurora Manzi, Christian Wolff, Jacek Stolarczyk, and Jochen Feldmann — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität Muenchen, Amalienstr. 54, D-80799

Solar hydrogen production is considered to be as one of the biggest challenges for future energy supply. Colloidal semiconductor nanoparticles, as sunlight absorber with additional noble metal nanoparticles as hydrogen catalyst are well known for photocatalytic hydrogen generation. Many of these systems suffer from low solar to hydrogen efficiencies unless high cost and rare materials like platinum or ruthenium compounds are used as co-catalysts. We demonstrate that it is possible to overcome all these problems with CdS nanorods with a very simple earth-abundant nickel-based co-catalyst. An apparent quantum yield exceeding 50% and long term stability of more than 200h could be achieved. We show that the photocatalytic activity is enhanced ten-fold in highly alkaline environment. Thanks to favourable band alignment the hydroxide anion acts as a redox shuttle relaying the hole from the nanocrystals. Since the hole transfer is considered to be the limiting factor, the quick hole scavenging at high pH is responsible for the enhancement of photocatalytic hydrogen evolution. [1]

[1] T. Simon, M.J. Berr, A. Vaneski, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk, J. Feldmann, submitted

HL 12.2 Mon 11:00 POT 081

Three-dimensional Ordered Macro-mesoporous Mo:BiVO4 Photoelectrode toward Efficient Photoelectrochemical Water Splitting — •Min Zhou[1,2], Yang Xu[1], Chengliang Wang[1], Liaoyong Wen[1], Yong Lei[1], and Yi Xie[2] — [1]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau, Germany — [2]University of Science & Technology of China, Hefei, China

In view of the worldwide energy challenge in the 21st century, the technology of semiconductor-based photoelectrochemical (PEC) water splitting has received considerable attention as an alternative approach for solar energy harvesting and storage.BiVO4 has been regarded as a promising material for PEC water splitting, but it suffers from a major challenge on charge migration. In order to meet this challenge, for the first time, we design a three-dimensional(3D) ordered macro-mesoporous architecture of Mo:BiVO4 through a controllable colloidal crystal template method. Within expectation, a superior photocurrent density is achieved in return for this design. This enhancement originates primarily from effective charge migration according to the analysis of electrochemical impedance spectroscopy. All the results highlight the great significance of the 3D ordered macro-mesoporous architecture as a promising photoelectrode model for the application in solar conversion. The cooperating amplification effects of nanoenegineering from composition regulation and morphology innovation provide new opportunities for creating more purpose-designed photoelectrodes with highly efficient performance.

HL 12.3 Mon 11:15 POT 081

Three-dimensional Composite Aerogels and Other Nanostructures for Improved Electrochemical Property — •Liying Liang[1,2], Yimeng Xu[1], Haimei Liu[1], and Yong Lei[2] — [1]Beijing University of Chemical Technology, State Key Laboratory of Chemical Resource Engineering, 100029 Beijing (PR China) — [2]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmenau (Germany)

Three-dimensional (3D) graphene aerogels possess a lot of unique properties, such as light weight, high conductivity, large surface area, high mechanical strength, and ample volume with hierarchically porous structure, which make them widely applied in various technological fields. Here, 3D porous composite aerogels have been synthesized via an innovative in situ hydrothermal method assisted by freeze-drying process. In this hybrid structure, one-dimensional (1D) AgVO3 nanowires are uniformly dispersed on two-dimensional (2D) graphene nanosheets surfaces or penetrate through the graphene sheets, forming 3D porous composite aerogels. The composite aerogels as cathode materials for lithium-ion batteries, exhibit high discharge capacity, excellent rate capability, and good cycling stability. We are also preparing more novel nanostructures by using AAO templates, which are expected to provide excellent electrochemical performance.

HL 12.4 Mon 11:30 POT 081

Three-dimensional Metal Oxides Based Nano-arrays Anodes for Sodium Ion Batteries — •Yang Xu, Min Zhou, Huaping Zhao, Chengliang Wang, and Yong Lei — Institute of Physics, Ilmenau University of Technology, 98693 Ilmenau, Germany,

The discovery of new materials/microstructures for electrodes in sodium ion batteries (NIBs) is receiving high levels of scientific attention, as sodium is substantially less expensive and more abundant than lithium. However, there is a limited choice of electrode materials that are suitable hosts to accommodate Na ions and allow for reversible insertion/extraction reactions, since Na ions are 55% larger in radius than Li ions. Of those, most have been identified to be potentially useful as cathodes. On the anode side, hard carbonaceous materials and insertion of Sn, Sb, Pb, and their alloys based anodes have been demonstrated to be highly promising. Another emerging class of materials that remains relatively unexplored in this case is conversion and/or insertion electrodes using transition metal oxides with reasonably low insertion potential. We report the successful utilization combining the nano-structured transition metal oxides and three-dimensional metallic current collector for NIBs anodes, and the results are demonstrated to be promising: the electrodes exhibited a highly stable reversible charge storage capacity over long term cycling, and were able to withstand high rate cycling with fully recovering the initial capacity. This proof-of-principle demonstration opens a way forward for future work on nano-architectures with better NIBs anode performance.

HL 12.5 Mon 11:45 POT 081

First principles study on the electronic properties of NaO_2 — •Markus Heinemann[1], Pascal Hartmann[2], Conrad L. Bender[2], Philipp Adelhelm[2], Jürgen Janek[2], and Christian Heiliger[1] — [1]I. Physikalisches Institut, Justus Liebig University, 35392 Giessen, Germany — [2]Physikalisch-Chemisches Institut, Justus Liebig University, 35392 Giessen, Germany

In the light of the recent discovery of rechargeable room-temperature sodium superoxide (NaO_2) batteries [1], a deeper understanding of the electronic properties of NaO_2 has become of broad interest. We investigate the electronic structure of NaO_2 using the framework of density functional theory and employ a hybrid functional approach for the exchange and correlation interaction. The disordered pyrite structure of the NaO_2 room-temperature phase is modeled by taking into account various superoxide orientations in our computations. Our band structure calculations indicate that NaO_2 is an insulator with an energy band gap in the range of 2 eV and that different superoxide alignments lead to a broadening of the conduction band. We compare our calculations to recent experimental investigations on the conductivity of NaO_2.

[1] P. Hartmann, C. L. Bender, M. Vračar, A. K. Dürr, A. Garsuch, J. Janek, and P. Adelhelm, Nature Mat. 3486, 1 (2012)

HL 12.6 Mon 12:00 POT 081

Photostability of GaN-metal interfaces in aqueous media — •Carina Ehrig[1,2], Ralf Krause[1], Christoph Brabec[2], and Günter Schmid[1] — [1]Siemens AG, CT RTC MAT IEC-DE, Erlangen — [2]Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik, FAU Erlangen-Nürnberg, Erlangen

Gallium nitride (GaN) is a well-established semiconductor in optoelectronic applications. It has a wide band gap of 3.4 eV and is thus excitable in the near UV range. A promising application of GaN is its use as a photo electrode driving electrochemical reactions such as photocatalytic water splitting for generation of hydrogen without consumption of fossil fuel or emission of CO_2. The corrosion resistance of those photo electrodes in aqueous media is one of the main factors determining their lifetimes and thus plays an important role for their applicability for highly efficient solar energy conversion. It has been demonstrated in photocatalytic experiments, that under UV-illumination n-type GaN acts as oxygen evolving photo anode and p-type GaN as hydrogen evolving photo cathode.

In the present work, the corrosion resistance of metal-coated n-GaN

and p-GaN photoelectrodes in aqueous media is investigated by electrochemical measurements. The influence of an externally applied potential under light excitation as well as the effect of long-term photo-induced stress are studied. It is observed that without illumination the GaN surfaces and GaN-metal interfaces are rather stable, whereas they undergo different corrosion processes when exposed to UV light.

HL 12.7 Mon 12:15 POT 081

Growth and characterization of 3D graphene networks for supercapacitors — •Simon Drieschner and Jose Antonio Garrido — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

The use of graphene as electrode material in supercapacitors has drawn great interest due to a suitable combination of material properties like high surface to volume ratio, high conductivity, and chemical stability. Since the capacitance of one single graphene sheet is rather limited, a continuous 3D network of graphene is expected to enhance the performance of graphene-based supercapacitors. We demonstrate the growth of 3D graphene by chemical vapor deposition (CVD) using a nickel foam as scaffold and a wet-etching transfer, yielding a free-standing macroporous graphene network of high crystalline quality, as shown by Raman spectroscopy. Cyclic voltammetry, charge-discharge measurements, and electrochemical impedance spectroscopy are used to assess the potential of 3D networks of CVD graphene for energy storage applications. We also compare the electronic double layer capacitance of bare graphene foam to the pseudo-capacitance introduced by conductive polymers.