HL 32: Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures I

Time: Tuesday 10:15–13:00 Location: POT 151

Invited Talk HL 32.1 Tue 10:15 POT 151

Self-assembled monolayers on zinc oxide — •Craig L. Perkins — National Renewable Energy Labooratory, Golden, CO USA — Renewable and Sustainable Energy Institute

Two of the most promising schemes for attaching organic molecules to metal oxides are based on the chemistry of the thiol and phosphonic acid moieties. We have made a direct comparison of the efficacy of these two molecular anchors on zinc oxide by comparing the chemical and physical properties of n-hexane derivatives of both. The surface properties of polycrystalline ZnO thin films and ZnO(0001)-O crystals modified with 1-hexanethiol and 1-hexanephosphonic acid were examined with a novel quartz crystal microbalance (QCM)-based flow cell reactor, angle-resolved and temperature-dependent photoelectron spectroscopy, and contact angle measurements. A means of using ammonium chloride as a probe of molecule-ZnO interactions is introduced and used to ascertain the relative quality of self-assembled monolayers (SAMs) based on thiols and phosphonic acids. QCM data shows that a phosphonic acid-anchored alkyl chain only six carbons long can provide significant corrosion protection for ZnO against Brønsted acids, reducing the etch rate relative to the bare ZnO surface by a factor of more than nine. The thermal stability of the two linking groups was also explored and we find that previous claims of highly stable alkanethiolate monolayers on ZnO are suspect. Taken as a whole, our results indicate that the phosphonic acid moiety is preferred over thiols for the attachment of short alkyl groups to ZnO.

Invited Talk HL 32.2 Tue 10:45 POT 151

Inorganic/organic semiconductor heteroepitaxy - towards new hybrid systems for optoelectronics and photonics — •Sylke Blumstengel — Institute of Physics, Humboldt University Berlin, Newtonstr. 15, 12489 Berlin

This talk summarizes our recent efforts to fabricate heterostructures based on ZnO and various conjugated organic materials as well as to tailor their electronic and optical properties. Growth by molecular beam epitaxy of both material components ensures well-defined interfaces and highest structural quality. A unique feature of ZnO and its ternaries ZnCdO and ZnMgO is that films and quantum structures with very good crystalline and optical properties can be epitaxially grown at low temperatures (50°C!) compatible with the stability of organic materials. Thus, not only organic-on-inorganic, but also inorganic-on-organic epitaxy can be performed. Relevant growth mechanisms are discussed. Interfacial energy level alignment including band-offset engineering via the geometric structure of the molecular layer is presented. Direct electronic coupling of the fundamental excitations (Frenkel and Wannier-Mott excitons) across the interface occurs with coupling constants on the meV-energy scale. The superior optoelectronic function of sandwich-type hybrids is demonstrated by the achievement of stimulated emission of the enclosed organic layer at markedly reduced pump thresholds due to efficient energy transfer from ZnO.

15 min. break

Invited Talk HL 32.3 Tue 11:30 POT 151

Electrostatic Field Driven Alignment of Organic Oligomers on ZnO Surfaces — •Fabio Della Sala[1], Sylke Blumstengel[2], and Fritz Henneberger[2] — [1]Nanoscience Institute (CNR), Via per Arnesano, 73100 Lecce — [2]Institut fuer Physik, Humboldt-Universitaet zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany

We present a theoretical study on the physisorption process of organic oligomers on the ZnO($10\bar{1}0$) surface. Using first-principles density-functional theory and non-empirical embedding methods, we find that both in-plane location and orientation of the molecules are completely determined by the coupling of their quadrupole moments to the periodic dipolar electric field present at the semiconductor surface. The adsorption is associated with the formation of a molecular dipole moment perpendicular to the surface, which bears an unexpected linear relation to the molecule-substrate interaction energy. Long oligomers such as sexiphenyl become well-aligned with stabilization energies of several 100 meV along rows of positive electric field, in full agreement with recent experiments. These findings define a new route towards the realization of highly-ordered self-assembled arrays of oligomers/polymers on ZnO($10\bar{1}0$) and similar surfaces.

Invited Talk HL 32.4 Tue 12:00 POT 151

The incorporation of metal nanostructures at organic/inorganic semiconductor interfaces — •Dietrich RT Zahn, Michael Ludemann, Ovidiu Gordan, Philipp Schäfer, and Georgeta Salvan — Semiconductor Physics, Chemnitz University of Technology, 09107 Chemnitz

Raman spectroscopy is applied in situ and online to study the interface formation of organic semiconductors such as perylene derivatives and phthalocyanines on inorganic semiconductor like gallium arsenide and silicon. Moreover, also the interface formation between metals and organic semiconductors has been extensively investigated. In the latter case the surface enhanced Raman scattering (SERS) effect is observed and it provides useful information regarding e.g. metal reactivity and metal diffusion. More recently well defined metal nanostructures were prepared on oxidised silicon samples using nanosphere lithography. When organic molecules are deposited onto such structured substrates strong enhancement effects are again observed. However, the enhancement effect shows an unusual resonance behaviour at excitation wavelengths well away from the metal cluster plasmon energy. The potential of such structures for application will be illuminated.

HL 32.5 Tue 12:30 POT 151

Fabrication of ZnO/polymer hybride devices using chemical vapor deposition of polymers — •Jan Richters and Tobias Voss — Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen

Due to their large surface area and good electrical conductivity, ZnO nanowires are interesting candidates for the fabrication of hybrid inorganic/organic optoelectronic devices. As an example, dye-sensitized solar cells can be prepared using a ZnO nanowire-array as one electrode with a monolayer of dye adsorbed on their surface. An additional hole-conductive material is required to form the connection with the counter electrode, where PEDOT:PSS or similar polymers can be applied. These polymer layers are usually fabricated using liquid-based synthesis-methods such as dip-coating or spin-coating which suffer from a limited penetration depth of the polymer into the pores of the nanowire array.
Here, we present a vapor-transport technique for the fabrication of dye-sensitized solar cells based on ZnO nanowires and the polymers PEDOT and polystyrene. We compare the electrical and optical properties of the devices, describe the microscopic properties of the polymer layers and provide details of the fabrication technique.

HL 32.6 Tue 12:45 POT 151

Electrical investigations of different polymer and substrate materials for dye-sensitized ZnO-NW/polymer hybrid solar cells — •Kay-Michael Günther[1], Julia Waltermann[1], Stefan Kontermann[2], and Wolfgang Schade[1,2] — [1]Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — [2]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, 38640 Goslar

Dye-sensitized solar cells composed of a n-doped ZnO nanowire (NW) array and a p-doped polymer layer appear to be a promising candidate for low-cost production of environment-friendly solar cells. In this study, we compare the commonly used polymer layers PEDOT:PSS and P3HT. While the former one provides a better conductivity, the latter one shows itself a photoabsorbance below $\lambda = 400$ nm. In addition, we investigate three different TCO substrates (ITO, FTO and ZnO:Al) using Impedance Spectroscopy (IS), current-voltage-measurements (IV), as well as IV-transients. The results show that in our setup an additional polycrystalline ZnO layer beneath the ZnO NWs is needed to prevent short circuits caused by polymer seeping between the NWs towards the counter electrode. Furthermore, the confinement to a simple ZnO layer enables us to optimize the polymer layer independently from the NWs. Hence, we compare devices with and without NWs and with different processing parameters. We achieve the best results with P3HT and FTO substrates. With ZnO:Al, we observe additional RC-combinations which partly result from a Schottky barrier formed at the ZnO:Al interface leading to a significant higher series resistance. An equivalent circuit is derived and discussed.