

O 30: Inorganic/Organic Interfaces: Towards Application

Time: Tuesday 14:00–16:00

Location: MA 043

O 30.1 Tue 14:00 MA 043

Increased light emission from organic light emitting diodes by surface plasmon polariton modification — ●CORNELIUS FUCHS¹, PAUL-ANTON WILL¹, MARTIN WIECZOREK¹, MALTE C. GATHER², SIMONE HOFMANN¹, SEBASTIAN REINEKE¹, KARL LEO¹, and REINHARD SCHOLZ¹ — ¹Technische Universität Dresden, Institut für Angewandte Photophysik, George-Bähr Str. 1, 01069 Dresden — ²University of St. Andrews, SUPA, School of Physics and Astronomy, North Haugh, St. Andrews, Scotland, UK, KY16 9SS

We demonstrate enhanced external quantum efficiency (EQE) from monochrome top-emitting light emitting diodes (OLEDs). The EQE is increased by about 20% compared to an optimized reference device. The enhancement is achieved by modifying the refractive index of the hole transport layer (HTL) material. The reference HTL possesses a refractive index of 1.77, averaged over the emission spectrum of the emitter material, whereas the improved device uses a HTL with a lower refractive index of 1.52. Both devices are optimized for maximized first order outcoupling efficiency. Due to the low refractive index of the HTL, the dispersion relation of the surface plasmon polariton (SPP) excited at the opaque metal bottom electrode shifts to smaller in-plane wavenumbers compared to the reference HTL. The shift decreases the power lost into evanescent excitations. Hence, the outcoupling efficiency of the OLED is increased, leading to the enhanced EQE. The proposed method is found to be applicable to emitter materials possessing isotropic as well as oriented distribution of the transition dipole moments.

O 30.2 Tue 14:15 MA 043

Charge Transport through Carbon Nanomembrane Molecular Junctions — ●PAUL PENNER¹, XIANGHUI ZHANG¹, EMANUEL MARSCHEWSKI¹, FLORIAN BEHLER², POLINA ANGELOVA¹, ANDRÉ BEYER¹, JENS CHRISTOFFERS², and ARMIN GÖLZHÄUSER¹ — ¹Fakultät für Physik, Universität Bielefeld, Bielefeld, Germany — ²Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Self-assembled monolayers (SAMs) of phenylthiol (PT), biphenylthiol (BPT), p-terphenylthiol (TPT) and p-quaterphenylthiol (QPT) formed on polycrystalline Au(111) are irradiated with low energy electrons and convert to carbon nanomembranes (CNMs). Molecular junctions incorporating pristine and cross-linked self-assembled monolayers (SAMs) from thiophenyl homologues are fabricated and investigated. A two-terminal setup composed of a Ga₂O₃/EGaIn top electrode and the Au substrate on which SAMs are prepared as a bottom electrode was used to characterize the molecular junctions. A comparison of charge transport characteristics reveals a decrease of conductance of CNM-based junctions by one order of magnitude, as well as a conversion of asymmetric junctions with SAMs into symmetric junctions with CNMs, which could be attributed to the decoupling of CNMs from the Au substrate and the partial loss of aromaticity of CNMs after irradiation. Transition voltage (TV) spectroscopy was also employed to investigate both types of junctions. We observe the length-dependent behavior of TV in both systems and a reduction of TV of CNM-based junctions in comparison to SAM-based junctions.

O 30.3 Tue 14:30 MA 043

Fabrication of (supra)molecularly precise 2D material device elements — ●SARAH WIEGHOLD², JUAN LI¹, MAXIMILIAN KRAUSE², PATRICK SIMON^{1,3}, JOSE GARRIDO^{1,3}, YURI AVLASEVICH⁴, CHEN LI⁴, KLAUS MÜLLEN⁴, UELI HEIZ², JOHANNES BARTH¹, CARLOS-ANDRES PALMA¹, and FRIEDRICH ESCH² — ¹Physik-Department, Technische Universität München, 85748 Garching, Germany — ²Chemie-Department, Technische Universität München, 85748 Garching, Germany — ³Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany — ⁴Max Planck Institute for Polymer Research, 55128 Mainz, Germany

The recent spotlight on highly crystalline natural-occurring and synthetic two-dimensional materials (2DMs) stands as a unique opportunity to accelerate atomically-precise technology. Here we explore the fabrication and characterization of 2D material devices of supramolecular networks with graphene attaining molecular precise disposition of all elements at interfaces. We present the first technologically relevant, photovoltaic response of a by-design artificial 2DM consisting

of a bicomponent supramolecular network on transparent, graphene-passivated H-C(100) diamond [1] and employing a gallium droplet as a counter electrode. Our results pave the way toward atomically precise (opto)electronic technology.

[1] Li, J. et al., Three-dimensional bicomponent supramolecular nanoporous self-assembly on a hybrid all-carbon atomically flat and transparent platform, *Nano Letters* 2014, 14, 4486.

O 30.4 Tue 14:45 MA 043

Reactive interaction of (sub-) monolayers and multilayers of the ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfanyl)imide with co-adsorbed lithium on Cu(111) — ●FLORIAN BUCHNER^{1,2}, MARAL BOZORGCHENANI^{1,2}, BENEDIKT UHL^{1,2}, HANIEH FARKHONDEH^{1,2}, and R. JÜRGEN BEHM^{1,2} — ¹Helmholtz Institute Ulm, 89081 Ulm, Germany — ²Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

The ionic liquid 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfanyl)imide [BMP][TFSA] is a promising candidate for the improvement of rechargeable Li-ion batteries. In this model study the reactive interaction of (sub-) monolayers and multilayers of [BMP][TFSA] with lithium (Li) was investigated on Cu(111) by scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIRS) under ultrahigh vacuum conditions. Upon co-deposition of Li to [BMP][TFSA] multilayers at 80 K we mainly identified changes in the chemical state of the [TFSA] anion and changes in absorption of anion related mid-IR bands. The co-deposition of Li to [BMP][TFSA] (sub-) monolayers verified the decomposition of [TFSA], independently on the order of deposition. After annealing to 300 K, most of the carbon of the anion and the cation desorbs; at 450 K LiF and Li₂S decomposition products dominate. Addition of very small amounts of Li to [BMP][TFSA] resulted in intriguing changes in the STM images which are most likely due to a surface mediated coordination of Li to [TFSA].

O 30.5 Tue 15:00 MA 043

Ultrathin Ionic Liquid Films on HOPG and on Ni(111)-supported graphene — ●FLORIAN RIETZLER¹, JENS NAGENGAST², HANS-PETER STEINRÜCK¹, and FLORIAN MAIER¹ — ¹Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — ²Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Profound knowledge of the interfaces between ionic liquids (ILs) and carbonaceous surfaces is highly relevant in catalysis and electrochemistry. In this work, ultrathin films of the IL 1,3-dimethylimidazolium bis(trifluoromethylsulfanyl)imide ([C1C1Im][TF2N]) were prepared under clean ultra high vacuum conditions by means of physical vapor deposition, and were analyzed by angle resolved XPS (ARXPS). The films were deposited onto highly oriented pyrolytic graphite (HOPG) as well-defined reference system, and onto nickel-supported graphene surfaces. Using ARXPS detailed information on the growth mode and on the molecular orientation of the IL is accessible.

For all investigated systems, clear evidence for three-dimensional growth was found. However, film morphology strongly depends on the nature of the substrate. In particular, the interaction of the IL with supported graphene seems to be stronger than with HOPG.

The results will be compared to ultrathin IL films deposited on well-defined metal surfaces such as Ni(111) and Au(111).

O 30.6 Tue 15:15 MA 043

Stability of thin layers of the ionic liquid [BMP][TFSA] on a rutile TiO₂(110) surface and co-deposition of Li — ●BENEDIKT UHL^{1,2}, MARAL HEKMATFAR^{1,2}, FLORIAN BUCHNER^{1,2}, DOROTHEA ALWAST^{1,2}, and R. JÜRGEN BEHM^{1,2} — ¹Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — ²Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

Ionic liquids (IL) have attracted high interest because of their special chemical and physical properties; among others, the application in electrolytes of Li-ion batteries is a promising concept. To gain a better understanding of the fundamental molecular processes

at the electrode|electrolyte interface, the interaction of n-butyl-n-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide [BMP][TFSA] with rutile $\text{TiO}_2(110)$ was investigated by X-ray photoelectron spectroscopy (XPS) in grazing emission and scanning tunneling microscopy (STM) under UHV conditions at temperatures between 80 K - 630 K. [BMP][TFSA] on $\text{TiO}_2(110)$ is stable and does not show decomposition up to around 470 K. Addition of Li, either before or after [BMP][TFSA] deposition, leads to a reaction of Li with the TiO_2 substrate and formation of a new Ti^{3+} species in the near surface region together with a new oxygen species. Thereby the [BMP][TFSA] stays intact, however, all its signals shift by roughly 1 eV to higher binding energies, which is most likely due to interactions with the new Ti^{3+} species in the substrate. Most important, the thermal stability of the [BMP][TFSA] is not affected by the Li-incorporation.

O 30.7 Tue 15:30 MA 043

Adsorption of organic molecules on a water-covered Fe(100) surface from first-principles — •GREGOR FELDBAUER^{1,2}, PEDRO BEDOLLA², MICHAEL WOLLOCH², PETER MOHN¹, JOSEF REDINGER¹, and ANDRÁS VERNES^{1,2} — ¹Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — ²Austrian Center of Competence for Tribology, Wiener Neustadt, Austria

Biofuels, especially ethanol mixed with standard gasoline or diesel, have become an important part of the worldwide motor fuel consumption. [1] Hence, the interaction of organic molecules constituting such biofuels with metallic surfaces is of high technological interest. In a combustion engine apart from organic molecules of the pure fuel there are always other chemical constituents, which may change the interfacial properties of the metallic surface. Water or acids contained in fuel lubricity additives and trace contaminants are prominent examples. In this contribution, the adsorption of ethanol, isooctane and acetic acid on a bare and a water-covered bcc Fe(100) surface is investigated within the framework of density functional theory including van der

Waals interactions. In particular, the impact of a water mono-layer on the adsorption energies, equilibrium configurations and electronic charge distributions is discussed. It is shown that the effect of the water layer strongly depends on the type of bond between the molecule and the surface. In addition, the possibility of a dissociative adsorption of the acetic acid and the formation of molecular hydrogen is studied.

[1] IEA, Tracking Clean Energy Progress 2013; International Energy Agency, Paris, 2013

O 30.8 Tue 15:45 MA 043

Modeling of air exposed titanium dioxide — WENKE FRIEDRICH, NORMAN GEIST, DENNIS SANDVOSS, and •WALTER LANGEL — Institut für Biochemie, Universität Greifswald, 17489 Greifswald

Adhesion of biomolecules to inorganic surfaces is of considerable interest for medical applications. We report a classical molecular dynamics study of peptides on titanium dioxide. Previous work refers to clean hydroxylated surfaces mimicking UHV-preparation. Air exposed Ti is not only passivated and partially hydroxylated but also covered by a hydrocarbon film making it more hydrophobic than a polar metal oxide. A computational model for this contamination must be based on volatile organic compounds in atmosphere, which screen the hydrophilic surface and are poorly soluble in water films on it. We report simulations of pentanol layers of various mass coverage on a variety of TiO_2 -surfaces. Physisorbed layers are stable, and their contact angles match experimental data. * On the clean hydroxylated surfaces most peptides easily adsorb in the simulation due to polar groups. In contrast to other work we can trace hindering of adsorption by the hydrocarbons working as a microscopic wax. Only partly hydrophobic species penetrate the contamination and attach due to polar groups, and this behavior seems to be correlated with the partition coefficient of the peptide. This result should have impact on several applications of titanium dioxide.