O 41: Poster: Metal Substrates - Structure, Epitaxy, Growth and Adsorption

Time: Tuesday 18:15–20:30 Location: Poster A

O 41.1 Tue 18:15 Poster A

Surface Chemical Bond of a Non-Alternant Aromatic Molecule on Metal Substrates — •Lukas Ruppenthal[1], Benedikt P. Klein[1], Nadine J. van der Heijden[2], Markus Franke[3], Claudio K. Krug[1], Stefan R. Kachel[1], Phil Rosenow[1], Francois Posseik[3], Martin Schmid[1], Ralf Tonner[1], Ingmar Swart[2], Christian Kumpf[3], and J. Michael Gottfried[1] — [1]FB Chemie, Philipps-Universität Marburg, Germany — [2]Debye Insitute, Utrecht University, The Netherlands — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany

Metal/organic interfaces have a large impact on the performance of organic-electronic devices, which makes their understanding an important target in surface science. Up to now, the focus has been almost exclusively on aromatic systems with alternant topology such as pentacene, which have a uniform charge distribution and highly delocalized frontier orbitals. In contrast, non-alternant aromatic systems have non-uniform charge distributions and more localized frontier orbitals. These properties are potentially interesting for organic electronics. In this contribution, we present a systematic study of the non-alternant aromatic molecule azulene on the (111) surfaces of Cu and Ag and compare it to its alternant counterpart naphthalene on the basis of NEXAFS, UPS, TPD, nc-AFM, STM and NIXSW measurements. Periodic DFT calculations confirm that the non-alternant topology results in much stronger interaction with metal surfaces, especially in the case of Cu(111), and that the resulting surface chemical bond is more localized.

O 41.2 Tue 18:15 Poster A

spontaneous formation of a superconductor-topological insulator $HfTe_3$ - $HfTe_5$ layered heterostructure — •yuqi wang[1,2], xu wu[1,2], ye-liang wang[1,4], shao yan[1], tao lei[3], jia-ou wang[3], shi-yu zhu[1], haiming guo[1], ling-xiao zhao[1], simin nie[1], hongming weng[1,4], kurash ibrahim[3], xi dai[1,4], zhong fang[1,4], and hong-jun gao[1,4] — [1]Institute of Physics, Chinese Academy of Sciences, Beijing, P. R. China — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, P. R. China — [4]Collaborative Innovation Center of Quantum Matter, Beijing, P. R. China

Recently, 2D materials and their heterostructures have shown unusual properties. In particular, $HfTe_5$ films and bulk $HfTe_3$ are reported to be 2D large-gap topological insulators (TIs) and superconductors (SCs), respectively. Such a heterostructure made of an s-wave SC and a TI is potentially suitable for studying amazing phenomena including Majorana Fermions. Here we report fabricating a SC-TI heterostructure with a layered configuration of $HfTe_3/HfTe_5$ [1]. The structure of the heterostructure has been determined by STM and XPS. STS measurements reveal a band-gap as large as 60 meV in the HfTe5 film and a SC spectrum in $HfTe_3/HfTe_5$ film. Our current method of making desired heterostructures is based on a spontaneous formation process using surface reactions. This method may provide new routes for the development of other functional heterostructures and nanodevices. References 1. Y. Wang et al., Adv. Mater, 28, 5013 (2016).

O 41.3 Tue 18:15 Poster A

IV-LEED investigations of Ag(001): experimental effects and data analysis — •Jascha Bahlmann, Frederic Timmer, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

IV-LEED is a powerful technique for surface sensitive structure analysis since the electrons of the used energy range provide information of only the few topmost surface layers. For a successful IV-LEED analysis, it is crucial to know the influences of the experimental setup like the angle of incidence of the electron beam or the temperature of the sample as well as the subtleties in data evaluation.

These effects were investigated systematically for the well known Ag(001) surface. Especially, we examined their influence on IV-curves recorded in the energy range 50-700 eV and studied the effect on the Pendry R-factor and the resulting geometrical structures determined by IV-LEED analysis. Low temperatures and a well known angle of incidence are essential for reliable results. Additionally the Debye-Waller factor and the root mean square of the thermal displacement of atoms were determined. Furthermore the influence of different filters for the smoothing of experimental spectra was evaluated.

O 41.4 Tue 18:15 Poster A

Investigation of Fe/W(110) system with Field Emission Scanning Probe Microscopy — •Robin Pröbsting[1], Gabriele Bertolini[1], Danilo Andrea Zanin[1], Hugo Cabrera[1], Urs Ramsperger[1], Danilo Pescia[1], and Oguzhan Gürlü[1,2] — [1]Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Istanbul Technical University, Department of Physics, 34469 Istanbul, Turkey

We studied the structural and electronic properties of atomic layer iron films on clean and carbide covered W(110) crystal surfaces. Surface structures were studied first by scanning tunnelling microscopy (STM). By means of retracting the tip several nanometres from the sample and increasing the tip bias with respect to the sample, we are able to measure field emitted current both on the tip and on the sample side of the junction. Also, secondary electrons (SE) generated on the sample were collected with a channeltron. Secondary electron maps of the surfaces acquired simultaneously with the absorbed current maps revealed that the local electronic nature of the iron-tungsten system is much richer than the STM shows. The nanometre lateral resolution attained in SE maps and the measurement of the image potential states on different surface locations presents the Topografiner as a potential candidate for atomic level spectroscopy on surfaces.

O 41.5 Tue 18:15 Poster A

Surface crystallography of large organic molecules on metal and insulator surfaces by LEED-IV using Fourier coefficients — •Ina Krieger[1,3], Georg Held[2], Christian Kumpf[3], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, 53115 Bonn, Germany — [2]Department of Chemistry, University of Reading and Diamond Light Source, UK — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52428 Jülich, Germany

We will report on LEED-IV analysis of the large organic molecules PTCDA and NTCDA on the metal and insulator surfaces Ag(100), Ag(111), and KCl(100). Using data from different angles of electron incidence and optimizing the LEED-IV program code we were able to extend the experimental data set and shorten the calculation times required for the complex and large unit cells. Furthermore, the distortion of the PTCDA molecule and the buckling of the Ag surface were described by Fourier coefficients taking into account the symmetry of the system [1]. The idea of this procedure is to suppress unphysical vertical displacements of atoms on a short-wave-length scale by restriction to lower order coefficients.

By this, we obtain good Pendry R-factors, for PTCDA/Ag100 of about 0.23. We were able to derive the vertical distortions of the oxygen atoms in the functional group and the buckling of the Ag surface in rather good agreement with earlier results from DFT and NIXSW studies.

[1] W. Moritz et al, Phys. Rev. Lett. 104, 136102 (2010).

O 41.6 Tue 18:15 Poster A

One-dimensional molecular chain of Co(TAP) on Au(111) — •Cen Yin — Peking university, beijing, China

combined scanning tunneling microscopy(STM), scanning tunneling spectroscopy (STS),) and tip molecular manipulation technique have employed to systematically explore on-surface properties of Co(TAP), as summarized in the following. On Au (111), the Co(TAP) molecules form two kinds of one-dimensional molecular chains. One is the bent chains that bend at the elbow points of the substrate and gradually disappear with the increase of its coverage. The other is the straight one-dimensional chains which adopt three specific surface orientations forming an obtuse angle of 120o against each other at low coverage. At high coverage, the straight molecular chains will not vanish. Variations of the assmeemblye structures with experimental conditions.On Au(111), the assembly structure is more seriously affected by temperature than by the coverage . At liquid nitrogen temperature, the Co(TAP) molecules form one-dimensional chains along the herringbone troughs eventually two-dimensional assembly structure at full coverage. On Ag (111), three co-existing assemblies the assembllies formed and are not affected by coverage and temperature. On Cu(111), the two-dimensional assembly structure appears only if the surface covrage reaches nearly full coverage.

O 41.7 Tue 18:15 Poster A

First principles investigations on the electronic structure of mercaptocarboxylic acids adsorbed on ZnO surfaces — •Dennis Franke[1], Michael Lorke[1], Andreia Luisa da Rosa[2], and Thomas Frauenheim[1] — [1]Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Universidade Federal de Minas Gerais, Dept. of Physics, Brazil

Scientific interest in devices consisting of organic and inorganic materials has grown over the past years. Such devices based on nanostructures are very sensitive to adsorbed compounds due to their large surface to volume ratios. In this work we investigate the electronic properties of mercaptocarboxylic acids (MPA) SH-$(CH_2)_n$-COOH adsorbed on ZnO-$(10\bar{1}0)$ surfaces via density functional theory calculations (DFT) using semi-local and hybrid exchange-correlation functionals. Previous DFT based results have shown that functionalizing the ZnO surface with a thiol group leads to molecular states inside the band gap. We find two possible binding modes for the thiol group on the surface, a monodentate and a bridge mode. We study the influence of both binding modes for different lengths of the methylene chain (n=1, 2, 4, 5, 7) on the density of states (DOS) and the dielectric function to draw conclusions about the possibility to tune the optical properties of ZnO nanostructures.