O 6: Poster Session I: Organic molecules on inorganic substrates: Adsorption and growth I

Time: Monday 10:30–12:30 Location: P

O 6.1 Mon 10:30 P

Graphene as an effective template for tuning the structural and electronic properties of organic-inorganic interfaces — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Controlling the morphological and electronic properties of organic-inorganic interfaces is essential for achieving efficient interface charge injection (or extraction) and transport properties in for example (opto)electronic devices. Here, we present a combined scanning tunneling microscopy and photoelectron spectroscopy study on the adsorption of 5,10,15,20-tetra(4-pyridyl)porphyrin (H2TPyP) on Cu(111) and graphene/Cu(111), respectively. Our experiments showed that for submonolayer coverage, H2TPyP does not form ordered 2D arrangements on Cu(111). Instead, the molecules adsorb randomly and adopt a saddle-shape configuration. However, annealing at 430 K results in short-range, ordered linear and triangular supramolecular arrangements stabilized by Cu-coordination. In contrast, for H2TPyP on graphene/Cu(111) a self-assembled 2D network stabilized by H-bonding forms with unit cell dimensions a = 2.7 nm, b = 1.2 nm and angle = 78°. Furthermore, the work function increases from 3.8 eV for H2TPyP/Cu(111) to 4.1 eV for H2TPyP/graphene/Cu(111), resulting in a considerably different energy level alignment at the hybrid interface. Our experiments demonstrate the feasibility of tuning organic-inorganic interface properties by employing graphene as an intermediate layer.

O 6.2 Mon 10:30 P

An organic electron donor on epitaxial graphene: the role of the metal support — •Joris de la Rie[1], Mihaela Enache[1], Qiankun Wang[1], Wenbo Lu[1], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute for Organic Chemistry, University of Heidelberg, Germany

Graphene has been the first of many 2D materials with excellent electronic properties which make it a material of great interest for future (nano)electronic devices. Implementation of graphene in devices requires interfacing graphene with other materials and tuning of the energy level alignment at the interface. The support on which graphene is placed affects its structural and electronic properties, and further modification is possible through the deposition of thin molecular films which have been shown to modify charge carrier type and concentration. Furthermore, the effect the support has on graphene (corrugation and doping) affects the molecular self-assembly and graphene-molecule interactions. Herein, we compare the self-assembly of an organic triphenylene-based donor (HAT) deposited on graphene on two supports: p doped graphene physisorbed on Ir(111) and n doped graphene chemisorbed on Ni(111). Using scanning tunneling microscopy and low energy electron diffraction we find that on both supports, HAT molecules assemble in a hexagonal network commensurate with the graphene lattice. We used X-ray and ultraviolet photoemission spectroscopy to study modifications of the electronic properties of graphene as well as intermolecular and molecular-graphene interactions.

O 6.3 Mon 10:30 P

Adsorption Behavior of Benzohydroxamic Acid on Rutile TiO_2(110) — •Julia Köbl[1], Elmar Kataev[1], Daniel Wechsler[1], Lisa-Marie Augustin[1], Nataliya Tsud[2], Stefano Franchi[2], Hans-Peter Steinrück[1], and Ole Lytken[1] — [1]University of Erlangen-Nürnberg, Erlangen, Germany — [2]Elettra-Sincrotrone Trieste, Trieste, Italy

Interfaces between organic molecules and oxide surfaces are present in many devices, such as dye-sensitized solar cells and organic field-effect transistors. The organic molecules are often covalently bonded to the oxide surface using specific anchor groups. Using synchrotron-radiation photoelectron spectroscopy, we will focus on how one of these anchor groups, hydroxamic acid, interacts with the rutile TiO_2(110)-(1x1) surface as a function of coverage, temperature, and deposition method. Hydroxamic acid is an interesting anchor group, because it is more stable than carboxylic acid, especially over a wide pH range, and more resistant towards hydrolysis. Benzohydroxamic acid can be evaporated intact in ultrahigh vacuum, and we will compare the behavior of both evaporated and solution-deposited molecules. Supported by the DFG through FOR 1878 (funCOS).

O 6.4 Mon 10:30 P

Chiral Recognition in the Self-Assembly of Trioxa[11]helicene on Metal Surfaces — •Bahaaeddin Irziqat[1], Jan Berger[1,2], Jesús Mendieta-Moreno[2], Mothuku Shyam Sundar[3], Ashutosh V. Bedekar[4], and Karl-Heinz Ernst[1,2] — [1]Surface Science and Coating Technologies, Swiss Federal Laboratories for Materials Science and Technology (EMPA), Dübendorf, Switzerland — [2]Nanosurf Laboratory, Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, The Czech Academy of Sciences, Prague, Czech Republic — [4]Department of Chemistry, The Maharaja Sayajirao University of Baroda, Vadodara, India

Chiral molecules adsorbed on metal surfaces have promising properties for applications in devices based on organic materials, such as chiroptical sensors or electron-spin filters. For this purpose, the two-dimensional (2D) crystallization of trioxa[11]helicene (TO[11]H) on the single crystalline (100) surfaces of Ag and Cu have been studied using scanning probe microscopy techniques (STM/nc-AFM) assisted by molecular dynamics simulations. In similarity to previously reported 2D-crystallization of heptahelicene ([7]H) on Ag(100) and Cu(100) [1,2], TO[11]H on Ag(100) shows a transition from homochiral structural motifs to large heterochiral domains with increasing coverage, whereas on Cu(100), enantiopure mirror domains, forming a 2D conglomerate structure, are observed.

O 6.5 Mon 10:30 P

Layer stability of porphyrin molecules on TiO2(110) — •Maximilian Muth, Alexander Wolfram, Elmar Kataev, Julia Köbl, Hans-Peter Steinrück, and Ole Lytken — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

Understanding the adsorption properties of organic molecules to substrate surfaces is of essential importance for applications. Typically, the adsorption energy of a smaller molecule to a surface can be determined by TPD. However, for large organic molecules only desorption of the multilayers is possible while the bottom monolayer in direct proximity to the surface cannot be desorbed without decomposition. But usually, especially the adsorption energies of these directly adsorbed molecules are the ones of the most interest. To overcome this problem we use a method including XPS with which we can determine the binding strength of differently metalated tetraphenyl porphyrins to a rutile TiO2(110) surface comparatively to each other. Therefore, a layer exchange between two differently metalated tetraphenyl porphyrins with subsequent desorption of the multilayers is caused by an annealing ramp. The composition of the residual monolayer is investigated by XPS. By using the ratios of the two porphyrins in the residual monolayer, we can estimate the difference in binding energy between the two porphyrins over a calculation of the equilibrium constant of the layer exchange process.

O 6.6 Mon 10:30 P

Adsorption energies of metalloporphyrins on MgO(100) — •Alexander Wolfram[1], Quratulain Tariq[1], Cynthia Fernandez[2], Bernd Meyer[3], Daniel Wechsler[1], Matthias Franke[1], Hans-Peter Steinrück[1], Federico Williams[2], and Ole Lytken[1] — [1]Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander Universität Errlangen-Nürnberg, GER — [2]Departamento de Química Inorgánica, Analítica y Química Física, Universidad de Buenos Aires, Ciudad Universitaria, ARG — [3]ICMM/CCC, Friedrich-Alexander-Universität Erlangen-Nürnberg, GER

Adsorption energies of large organic molecules on surfaces are often not well known. Experimentally, the large molecules are prone to decomposition before desorption, often ruling out desorption-based techniques. Theoretically, van der Waals interactions, which dominate the interactions between the molecules and the surface, are still challenging. However, for tetraphenylporphyrin adsorbed on MgO(100) desorption of the monolayer is possible, and, using simple Redhead analysis, we have extracted the desorption energies of cobalt, zinc, and magnesium tetraphenylporphyrin. Redhead analysis requires the prefactor for desorption to be known, and we have estimated this prefactor by a combination of transition-state theory and experimentally-derived prefactors from multilayer desorption. The resulting desorption energies are in good agreement with density functional theory calculations. Somewhat unexpectedly, CoTPP exhibits the lowest desorption energy and MgTPP the highest. We suggest the different oxophilicities of the metal centers to be the reason for the trend in adsorption energy.

O 6.7 Mon 10:30 P

Structural Investigation of Caffeine Monolayers on Au(111) — Malte G.H. Schulte[1,2], Andreas Jeindl[3], •Julian A. Hochhaus[1], Ismail Baltaci[1,2], Marie Schmitz[1,2], Ulf Berges[1,2], Oliver T. Hofmann[3], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, D-44227, Dortmund, Germany — [2]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227, Dortmund, Germany — [3]Institut für Festkörperphysik, NAWI Graz, Technische Universität Graz, Petersgasse 16, A-8010 Graz

In this study, we investigate caffeine monolayers on Au(111). The asymmetric and achiral structure of the caffeine molecule leads to two surface chiralities, which influence the crystal growth of caffeine. Knowledge of these structural properties is of interest because of the in- fluence of caffeine on the human central nervous system.

Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and X-ray photoelectron spectroscopy (XPS) were used to determine the structure of adsorbed caffeine. Additionally performed density functional theory (DFT) calculations allowed a conclusive interpretation of the results. We observed that the caffeine molecules adsorbed in a quasi-hexagonal formation resembling the high-temperature α phase and comprising two domains. The DFT calculations suggest a unit cell containing three molecules. The theoretically calculated structure is in excellent agreement with the experimentally measured LEED, STM and XPS data. The results are published in Phys. Rev. B **101**, 245414 (2020).

O 6.8 Mon 10:30 P

Validation of the inverted adsorption structure for free-base tetraphenyl porphyrin on Cu(111) — Paul TP Ryan[1,2], Paula Laborda Lalaguna[1,3], Felix Haag[4], Mona M Braim[5], Pencheng Ding[5,6], David J Payne[2], Johannes V Barth[4], Tien-Lin Lee[1], D Phil Woodruff[5], Francesco Allegretti[4], and •David A Duncan[1] — [1]Diamond Light Source, Didcot, UK — [2]Imperial College London, UK — [3]University of Glasgow, UK — [4]Technical University of Munich, Germany — [5]University of Warwick, Coventry, UK — [6]Harbin Institute of Technology, China

Utilising normal incidence X-ray standing waves we rigourously scrutinised the ”inverted model” as the adsorption structure of free-base tetraphenyl porphyrin on Cu(111). We demonstrate that the iminic N atoms are anchored at near-bridge sites on the surface, displaced laterally by 1.1*0.2Å in excellent agreement with previously published calculations, thus confirming that this unusual structure is indeed present on the surface.

O 6.9 Mon 10:30 P

Fabrication of high-quality 2-dimensional material single crystal nanoribbon networks — •Muhammad Awais Aslam[1], Markus Kratzer[1], Christian Teichert[1], Raul David Rodriguez[2], and Aleksandar Matković[1] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Tomsk Polytechnic University, Tomsk, Russia

We demonstrate an approach to synthesize 2D material nanoribbon networks. The epitaxially grown organic nanostructures align predominantly in either zig-zag or armchair orientation on 2D materials. 1,2 This study demonstrates their usage as a mask. These hybrid heterostructures are plasma etched to form single crystal nanoribbon networks. Raman spectroscopy and atomic force microscopy are employed to verify the quality of the ribbons. Our method opens up a new avenue for straightforward production of 2D material nanoribbon networks on scales relevant to electronic applications. Their high edge-to-surface ratios will also be of technological relevance for the development of future light and chemical sensors.

1.Kratzer, Teichert, 2016. Nanotechnol. 27, 292001.

2.Kratzer, Matkovic, Teichert, 2019 LPD, 52,383001.