O 102: Poster Session VIII: Organic molecules on inorganic substrates: electronic, optical and other properties IV

Time: Thursday 13:30–15:30 Location: P

O 102.1 Thu 13:30 P

Measuring the Change in Reactivity of a Single Molecule — •Jack Henry, Phil Blowey, and Adam Sweetman — University Of Leeds, Leeds, United Kingdom

Decades of surface science studies on adsorbed molecules have shown the surface a molecule is adsorbed on can effect the molecules electronic and geometric structure [1-3]. In this work, the influence of molecule-substrate bonding on the interactions experienced by a scanning probe microscope (SPM) tip were investigated.

A system comprised of C_{60} molecules adsorbed on the Cu(111) surface was studied using simultaneous non-contact atomic force microscopy (NC-AFM) and scanning tunnelling microscopy (STM). This system is ideal for invesitgating the effect molecule-substrate bonding has on the physico-chemical properties of a molecule as the C_{60}-Cu(111) interface can be controlled to form two distinct structures [4-6]. The physico-chemical properties of the C_{60} molecules were investigated using NC-AFM spectroscopy. A comparison was made by looking at the force minima in collected spectra, along with the corresponding junction conductance. Complementary ab initio simulations of the spectra were performed in density functional theory (DFT) to gain a deeper understanding of the experimental results.

[1] L. Gross et al. Science 325, 110 (2009); [2] J. Repp et al. PRL 94, 026803 (2005); [3] F Mohn et al. University Of Regensburg (2012); [4] W. Wu Pa et al. PRL 104, 036103 (2010); [5] J. A. Larsson et al. PRB 77, 115434 (2008); [6] J. Brand et al. Nano.Lett. 19, 7845-7851 (2019);

O 102.2 Thu 13:30 P

Identifying the Origin of Local Flexibility in a Carbohydrate Polymer — •Kelvin Anggara[1], Yuntao Zhu[2], Giulio Fittolani[2,4], Yang Yu[2], Theodore Tyrikos-Ergas[2,4], Martina Delbianco[2], Stephan Rauschenbach[1,3], Sabine Abb[1], Peter Seeberger[2,4], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research — [2]Max Planck Institute for Colloids and Interfaces — [3]University of Oxford — [4]Freie Universität Berlin — [5]École Polytechnique Fédérale de Lausanne

Correlating structures and properties of a polymer to its monomer sequence is key to understand how its higher hierarchy structures are formed and how its macroscopic material properties emerge. Carbohydrate polymers, such as cellulose and chitin, are the most abundant materials found in nature whose structures and properties have only been characterized at sub-micrometer level. Here, by imaging single cellulose chains at nanoscale, we determine the structure and local flexibility of cellulose as a function of its sequence (primary structure) and conformation (secondary structure). Changing the primary structure by chemical substitutions and geometrical variations in the secondary structure allow the chain flexibility to be engineered at the single linkage level. Tuning local flexibility opens opportunities for the bottom-up design of carbohydrate materials.

O 102.3 Thu 13:30 P

CoTPP molecules deposited on passivated Fe-(100)-p(1x1)O: a photoemission tomography study — •David Janas[1], Henning Sturmeit[1], Iulia Cojocariu[2], Vitaliy Feyer[2], Stefano Ponzoni[1], Giovanni Zamborlini[1], and Mirko Cinchetti[1] — [1]Experimentelle Physik VI, TU Dortmund, Otto-Hahn-Straße 2, 44227 Dortmund, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Leo-Brandt-Straße, 52425 Jülich, Germany

In order to enhance the performances of organic spintronic devices, a detailed knowledge of the physical properties at the interface is crucial [1]. In this context, photoemission tomography (PT), which combines ab-initio calculations and angle-resolved photoelectron spectroscopy (ARPES), stands out as a powerful tool to unravel the orbital structure of molecular thin films at metal/organic interfaces [2].

In our work we apply PT to investigate the interaction of paramagnetic molecules, namely CoTPP, on the passivated Fe-(100)-p(1x1)O surface. Recently, it was shown that the interactions at this interface lead to an emergent magnetic ordering of the molecular layer. Here, we use PT to further characterize this intriguing system. In particular, we precisely determine the energy level alignment at the interface, the nature of the frontier orbitals, and the azimuthal orientation of the CoTPP with respect to the substrate.

[1] Cinchetti, M., Dediu, V. & Hueso, L. Activating the molecular spinterface. Nature Mater 16, 507-515 (2017)

[2] Puschnig, P. et al. Reconstruction of molecular orbital densities from photoemission data. Science 326, 702-706 (2009)

O 102.4 Thu 13:30 P

Orientation Dependent Charge Transfer: Heptacene on Coinage Metals — •Andreas Windischbacher[1], Thomas Georg Boné[1], Marie Sophie Sättele[2], Holger F. Bettinger[2], Heiko Peisert[2], Thomas Chassé[2], Georg Koller[1], and Peter Puschnig[1] — [1]University of Graz, Graz, Austria — [2]University of Tübingen, Tübingen, Germany

Over the past decade, pi-conjugated, aromatic molecules have gained increased attention in material science as their electron donating or accepting nature can be exploited to tune the charge rearrangement in hybrid organic-inorganic systems. Major research efforts have been directed towards the description of effects related to this electron transfer between a surface and its adlayer, often focusing on the metal's work-function and the adsorbate's electron affinity.

In our contribution, we want to demonstrate the decisive impact of the adsorbate orientation on the charge transfer properties of a molecule-metal interface. We utilize density functional calculations to simulate the adsorption of heptacene, seven linearly fused benzene rings, on coinage metal surfaces M(110), M=Ag, Cu. Considering various adsorption configurations and unit cells, we elucidate the electronic structures of our systems, observing an unusually strong dependence on the orientation of the molecule. Complementary photoemission experiment data confirm the theoretical predictions.

O 102.5 Thu 13:30 P

SF-IETS studies on CuCu4(shi)4 metallacrown complex — •Robert Ranecki[1], Stefan Lach[1], Angeliki Athanasopoulou[2], Eva Rentschler[2], and Christiane Ziegler[1] — [1]Dept. of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Inst. of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, Germany

Exchange coupled magnetic centers on surfaces are expected to provide an excellent platform for the development of spintronic technologies. For such structures, the detection of spin excitations by low-temperature scanning tunnelling spectroscopy has enabled investigations on coupling individual spins [2]. Up to now, however, only a few Spin-Flip Inelastic Tunneling Spectroscopy (SF-IETS) measurements have been performed on single molecules encapsulating several spin centers [1]. Here, we present Scanning Tunneling Spectroscopy (STS) studies on an electrospray deposited 12-MC-4 metallacrown pentacopper(II) nanomagnet. We observe symmetric around zero-bias features on differential conductance spectra, an evident hallmark of inelastic tunneling. We use third-order electron transport model [2], assuming exchange coupling constants determined by the broken symmetry approach [3], to describe the experimental spectra. The obtained results provide access to intramolecular coupling of spins in a single molecular system with competing superexchange interactions.

[1] S.Kahle, et al. Nano letters 12, 518-521 (2012).

[2] M.Ternes, et al. J. Phys. Condens. Matter 21 053001 (2009).

[3] Y.Pavlyukh et al. Phys. Rev. B 99 144418 (2019).

O 102.6 Thu 13:30 P

Time-resolved orbital imaging of the CuPc/$TiSe_2$ interface — •Kiana Baumgärtner[1], Markus Scholz[2], Christian Metzger[1], Dmytro Kutnyakhov[3], Nils Wind[4], Michael Heber[3], Lukas Wenthaus[3], Kai Rossnagel[3,5], and Friedrich Reinert[1] — [1]Experimentelle Physik 7, Universität Würzburg, Germany — [2]European XFEL, Germany — [3]DESY, Hamburg, Germany — [4]Universität Hamburg, Germany — [5]Universität Kiel, Germany

In the last decade [1], the interpretation of the momentum distribution from static angle-resolved photoemission experiments has improved our understanding of charge transfer processes at the molecule-substrate interface [2] as well as the geometric alignment in these systems [3]. In this contribution I will present our experimental findings on time-resolved orbital imaging of the excited CuPc/$TiSe_2$ interface which were conducted at a HHG-laser facility with a momentum microscope. Previous studies on the transition-metal dichalcogenide $TiSe_2$ have shown exciting electronic behavior on the fs to ps time scale upon optical excitation [4]. With the introduction of CuPc as a charge donor new interaction channels arise at the interface and showcase the electronic as well as structural interplay at the interface. [1] P. Puschnig et al., Science 326, 702 (2009). [2] G. Zamborlini et al., Nat. Comm. 8, 335 (2017). [3] M. Grimm et al., Phys. Rev. B 98, 195412 (2018). [4] T. Rohwer et al., Nature 471, 490 (2011).

O 102.7 Thu 13:30 P

A multifunctional organic interface: decoupling the spin tuning from molecule-metal hybridization — •H. Sturmeit[1], I. Cojocariu[2], M. Jugovac[2], A. Windischbacher[3], P. Puschnig[3], C. Piamonteze[4], A. Sala[5,6], G. Comelli[5,6], A. Cossaro[5], A. Verdini[5], L. Floreano[5], M. Stredansky[5,6], E. Vesselli[5,6], C. Hohner[8], M. Kettner[8], J. Libuda[8], C. M. Schneider[2,7], G. Zamborlini[1], M. Cinchetti[1], and V. Feyer[2,7] — [1]TU Dortmund, Dortmund, Germany — [2]Forschungszentrum Jülich, Jülich, Germany — [3]Karl-Franzens-Universität, Graz, Austria — [4]Paul-Scherrer-Institute, Villigen, Switzerland — [5]Lab. TASC IOM-CNR, Trieste, Italy — [6]University of Trieste, Trieste, Italy — [7]Universität Duisburg-Essen, Duisburg, Germany — [8]Friedrich-Alexander-Universität, Erlangen, Germany

The possibility to separately address and control the spin and charge properties at a metal/organic interface could pave the way to a new generation of multifunctional devices. Here, by using a theoretical and experimental spectro-microscopy approach, we introduce a system with decoupled, and therefore independently tunable, spin and electronic properties. A single layer of nickel tetraphenyl porphyrin molecules strongly interacts with the copper (100) surface, causing a massive charge transfer and the uncommon Ni(I) oxidation state. We find that by dosing nitrogen dioxide (NO_2) the Ni(II) oxidation state of the gas phase molecule can be restored while the substrate-induced high-spin configuration is preserved.

O 102.8 Thu 13:30 P

SF-IETS studies on CuCu4(shi)4 metallacrown complex — •Robert Ranecki[1], Stefan Lach[1], Angeliki Athanasopoulou[2], Eva Rentschler[2], and Christiane Ziegler[1] — [1]Dept. of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Inst. of Inorganic and Analytical Chemistry, Johannes Gutenberg University Mainz, Germany

Exchange coupled magnetic centers on surfaces are expected to provide an excellent platform for the development of spintronic technologies. For such structures, the detection of spin excitations by Low-Temperature Scanning Tunnelling Spectroscopy (LT-STS) has enabled investigations on coupling individual spins [1]. Up to now, however, only a few Spin-Flip Inelastic Tunneling Spectroscopy (SF-IETS) measurements have been performed on single molecules encapsulating several spin centers [2]. Here, we present LT-STS studies on an electrospray deposited 12-MC-4 pentacopper(II) metallacrown system. We observe symmetric around zero-bias features on differential conductance spectra, an evident hallmark of inelastic tunneling. We use third-order electron transport model [1], assuming exchange coupling constants determined by the broken symmetry approach [3], to analyze our experimental data. The obtained results provide access to intramolecular coupling of spins in a single molecular system with competing superexchange interactions.

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