O 80: Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties I

Time: Thursday 10:30–12:30 Location: H4

O 80.1 Thu 10:30 H4

CISS in single heptahelicene molecules on Fe bilayers on W(110) — •Daniel E. Bürgler[1], Mohammad Reza Safari[1], Frank Matthes[1], Karl-Heinz Ernst[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut, Forschunschungszentrum Jülich, Germany — [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600, Dübendorf, Switzerland

We reproduce and extend our single-molecule studies of CISS [1,2] to an alternative substrate system. Heptahelicene molecules are sublimed onto a multi-domain Fe bilayer film on W(110) instead of single-domain Co bilayer nanoislands on Cu(111). Using spin-polarized low-temperature scanning tunneling microscopy, the current flow through single *(M)*-enantiomers chemisorbed on neighboring and oppositely magnetized domains of the Fe bilayer film is mapped in the constant-height mode, where the tip is scanned at constant height above the Fe surface. The CISS magnetoresistance reaches up to 18% at 5 K and shows a strong dependence on the bias voltage. A comparison is drawn with the data obtained on Co nanoislands.

[1] M.R. Safari, F. Matthes, V. Caciuc, N. Atodiresei, C.M. Schneider, K.-H. Ernst, D.E. Bürgler. Adv. Mater. **36**, 2308666 (2024)
[2] M.R. Safari, F. Matthes, C.M. Schneider, K.-H. Ernst, D.E. Bürgler, Small **20**, 2308233 (2024)

O 80.2 Thu 10:45 H4

STM topography and photoluminescence of three different Eu complexes — •Adrian Ebert[1], Lukas Gerhard[1], Julia Feye[2], Senthil Kumar Kuppusamy[3], Mario Ruben[3], Peter Roesky[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Organic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

We explore the self-assembly and luminescence properties of three distinct Europium (Eu) complexes *$\mathrm{Eu(tta)_3(H_2O)_2}$, $\mathrm{Eu(btfa)_3(bpy)}$, and $\mathrm{Eu(tta)_3(bpy)}$ * on a Au(111) surface. Utilizing Scanning Tunneling Microscopy (STM), we explore the molecular topography and the ordered structures formed by these complexes, providing insight into their surface interactions. The Europium $\mathrm{Eu^{3+}}$ ion, a member of the lanthanide series, is renowned for its unique photophysical properties, particularly its sharp emission lines and long-lived luminescence, which make it a valuable component in light-emitting devices, bio-imaging, and sensing applications.

O 80.3 Thu 11:00 H4

First-Principles Modeling of Mixed-Dimensional Heterostructures: A Path Forward — •Jannis Krumland and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg

Inorganic/organic interfaces between transition-metal dichalcogenides and organic adsorbates are promising candidates for future optoelectronic applications, leveraging and combining the unique strengths of the two different types of materials. The first-principles description of such interfaces, however, remains challenging because methods based on density-functional theory are unreliable for their simulation [1]. This is a result of the mixed dimensionality of the interface, with molecules being zero-dimensional while surfaces are two-dimensional. The mixed dimensionality moreover poses challenges in the analysis of the results, as molecules are usually described in terms of energy levels, whereas surfaces are characterized by band structures. Here, we present a methodological study establishing pragmatic yet accurate simulation approaches for the calculation of energy-level alignments [2]. In addition, we highlight unfolding techniques as a key tool for gaining a deeper understanding of the interactions and hybrid-state formation occurring at such interfaces [3].

[1] J. Krumland and C. Cocchi, Phys. Stat. Sol. A 221, 2300089 (2024)

[2] J. Krumland and C. Cocchi, J. Phys. Chem. Lett. 15, 5350-5358 (2024)

[3] J. Krumland and C. Cocchi, Electron. Struct. 3, 044003 (2021)

O 80.4 Thu 11:15 H4

Photo-induced force microscopy of organic molecules on thin van der Waals substrates — •Markus Kratzer[1], Mohamad Khan[1], Simon Leitner[1], Aleksandar Matkovic[1], Olivier Siri[2], Conrad Becker[2], and Christian Teichert[1] — [1]Chair of Physics, Montanuniversität Leoben, Franz-Josef Straße 18, 8700 Leoben, AUT — [2]Aix Marseille Univ., CNRS, Cinam, 13288 Marseille, FGrance

Photo-induced force microscopy (PiFM) is an atomic force microscopy based technique for obtainiung infrared spectroscopic data with a spatial resolution down to a few 10 nm. Here, we utilized PiFM to investigate nano and microstructures comprising small organic molecules like para-hexaphenyl or dihydro-tetraaza-acene (DHTA7) on exfoliated thin layers of van der Waals materials as hexagonal boron nitride (hBN). It is notices that the PiFM spectra systematically vary with van der Waals substrate thickness. Further PiFM spectra of upright standing molecular structures and flat lying structures are copared. PiFM turned out to be sensitive even for single molecular layers, which are only about 2 nm thick. Similarities and differences between thin film and bulk infrared data are discussed.

O 80.5 Thu 11:30 H4

Engineering Optical Properties through Polymorphism — •Nina Kainbacher[1,2], Peter Puschnig[1], and Oliver T. Hofmann[2] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Austria

Molecular monolayers on a supporting substrate can order in different configurations, i.e. polymorphs. Owing to variations of the intermolecular coupling between the transition dipole moments, we expect that different polymorphs exhibit also distinctly different optical properties due to changes in transition energies and oscillator strengths. In this study, we computationally study the impact of polymorphism of organic molecular monolayers on optical absorption spectra. Specifically, we investigate influencing factors, such as geometric distortions upon adsorption, interactions between transition dipole moments, changing selection rules due to the symmetry of different polymorphs, and particularly, effects arising from the potential delocalization of the wave functions. As an example, we predict the polymorphism of the dipolar organic molecule nitro-pyrene-amine on NaCl(100) using machine learning-based structure search and calculate its optical properties based on density functional theory and the RPA approximation. Specifically, we find two distinctly different polymorphs, where the excitation energies differ by approximately 0.2 eV which we attribute to a combination of the above-mentioned effects.

O 80.6 Thu 11:45 H4

Imaging the occupied states of multilayers of α-sexitiophene (6T) on Cu(110)-p(2x1)O using orbital tomography — •Monja Stettner[1,2], Andrey Matetskiy[1], Eric Fackelman[1,2], Siegfried Kaidisch[3], Serguei Soubatch[1], François C. Bocquet[1], Peter Puschnig[3], Christian Kumpf[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), FZ Jülich, Germany — [2]RWTH Aachen University, Germany — [3]Institute of Physics, University of Graz, Austria

Deposition of α-sexithiophene (6T) on an oxygen-reconstructed Cu(110)- p(2x1)O surface results in a well ordered, close-packed monolayer structure, and at higher coverages in layer-by-layer growth. Note that even beyond a monolayer, 6T retains its orientation along the [001] direction of Cu. We investigated samples with coverages of up to eight layers using ARPES and - in particular - orbital tomography. For the latter, experimental momentum maps are compared to simulated maps which are calculated for a single free molecule and for extended layers of 6T. We found a good resemblance for several occupied molecular states, e.g., the HOMO. However, in the binding energy range of several deeper orbitals, the momentum maps clearly show signatures of a sizable intermolecular dispersion that cannot be explained by a superposition of the single gas phase maps. The orbitals rather form dispersing bands, which indicates a significant intermolecular hybridization.

O 80.7 Thu 12:00 H4

Electronic structure of molecular and crystalline benzene on an $\mathrm{MoS_2}$ monolayer — •Jan-Phillip Topmöller and Michael Rohlfing — Institute of Solid State Theory, University of Münster,

Germany

TMDCs show great potential in terms of their applicability in optical electronics. Due to their large surface, molecules can easily bind to the TMDC and affect its electronic properties. Here we investigate molecular benzene and its bulk crystal as prototypical systems.

We use DFT (GGA) and DFT-D3 to determine the most stable adsorption position of both the molecule and the bulk crystal on MoS_2. Subsequently, we use many body perturbation theory to calculate the electronic spectrum of the adsorbate system and its individual components (MoS_2 and the benzene molecule/crystal) in order to investigate the effect of the molecule on the MoS_2 electronic and optical spectrum.

O 80.8 Thu 12:15 H4

Contact-dependent electronic properties of anthracene-MoS_2 heterostructures — •Hsin-Mei Ho and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Flexible nanodevices composed of atomically thin layers have revolutionized fundamental and applied sciences. Based on density functional theory (DFT), we consider the organic-inorganic heterostructures: anthracene molecules adsorbed on monolayer MoS_2. Our investigations of the adsorption geometries and the energy band dispersions demonstrate that the contact between the organic and inorganic layers greatly affects the electronic properties. Anthracene thin films give rise to different shifts of the frontier energy levels, and consequently, variations in the band alignments when the molecules are in the perpendicular and parallel orientations on MoS_2. As anthracene is known for ordered structures when grown on substrates, we find in the present study that the bandgap of an anthracene film reduces when the interactions between molecules increase. This suggests that how the molecules are packed also plays a critical role. Our study provides detailed insights regarding the advances of oligoacene-TMDs layers for both theoretical and experimental sides.