O 69: Nanostructures at surfaces:1D, 2D, networks – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 69.1 Wed 18:00 P2

Study of different structural phases of Ni-DCA networks on graphene/Ir(111) — •Ayesha Jabeen[1], Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Anna Kurowska[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic

2D metal-organic frameworks (MOFs) represent a promising class of two-dimensional nanomaterials with tunable electronic and magnetic properties, which could have potential applications in catalysis and spintronics. In this study, we investigate the structural phases and thermal stability of Ni-DCA (9,10-dicyanoanthracene) networks supported on graphene/Ir(111). Employing Low-Energy Electron Microscopy (LEEM), Scanning Tunnelling Microscopy (STM), and X-ray Photoemission Spectroscopy (XPS), we identified three distinct structural phases: two phases composed of isolated $Ni_1(DCA)_3$ coordination complexes coexisting with hydrogen-bonded DCA molecules, and one extended metal-organic framework with $Ni_2(DCA)_3$ stoichiometry. Despite their different long-range order, all three phases have the same local Ni coordination environment. Thermal annealing reveals that the $Ni_2(DCA)_3$ network is the least stable of the three, dissociating into the individual complex phases upon mild annealing around 80 °C. These findings elucidate the polymorphic nature and thermal limitations of Ni-DCA networks supported on graphene/Ir(111), contributing to the understanding of DCA-based MOFs.

O 69.2 Wed 18:00 P2

Examining the character of coordination bonding in two-dimensional MOFs by photoemission tomography — •Dominik Brandstetter[1], Simone Mearini[2], Andreas Windischbacher[1], Yan Yan Grisan Qiu[2], Daniel Baranowski[2,3], Vitaliy Feyer[2,4], Claus Micheal Schneider[2,4,5], and Peter Puschnig[1] — [1]University of Graz, Graz, Austria — [2]Jülich Research Centre, Jülich, Germany — [3]Present address: Pacific Northwest National Laboratory, Richland WA, USA — [4]University of Duisburg-Essen, Duisburg, Germany — [5]UC Davis, Davis CA, USA

We investigate the nature of the coordination bonds in 2D MOFs by examining a well-ordered nickel tetracyanoquinodimethane (Ni-TCNQ) monolayer on a Ag(100) substrate. Notably, photoemission data shows a splitting of the valence band into bonding and anti-bonding states, resulting from the interaction between the Ni d-states and the ligand orbitals. By making use of the energy-resolved photoemission momentum maps, we are able unambiguously reveal signatures of covalent bonding between the organic ligands and the transition metal d-states by identifying fingerprints of the involved orbitals in momentum space. These hybridized states are crucial in understanding the MOF's electronic structure, which is a determining factor for their electronic and magnetic properties. Our results are concrete evidence of the covalent character within 2D MOFs, offering a deeper understanding of their fundamental electronic properties.

O 69.3 Wed 18:00 P2

Superconducting quantum corrals — •Divya Jyoti[1] and Nicolás Lorente[2] — [1]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]Centro de Fisica de Materiales (CFM), Donostia - San Sebastian, Spain

Quantum corrals enable atomically precise control of electronic confinement on surfaces, and their extension to superconductors opens new possibilities for manipulating in-gap Bogoliubov quasiparticles. In this work, we develop a microscopic Bogoliubov-de-Gennes Green-function framework [1-2] for multiple δ-like impurities on 2D superconducting lattices. As a benchmark, the method reproduces the superconducting mirage associated with Yu-Shiba-Rusinov states in elliptical corrals. By tuning the corral geometry, and material parameters, the spatial structure and spectral evolution of in-gap quasiparticle states is determined. We further explore the effect of confinement on engineered topological phases by placing a Majorana-hosting ferromagnetic spin chain inside an elliptical corral and showing that geometric confinement strongly hybridizes its zero-energy modes, redistributing their spin texture and shifting spectral weight to finite energies. These confined in-gap states offer a new route to engineer topological features, linking atomically crafted quantum matter to emerging platforms for topological quantum computation. [1] Morr et al., Phys. Rev. Lett. 92, 107006 (2004) [2] Flatté et al., Phys. Rev. B 56, 11213 (1997)

O 69.4 Wed 18:00 P2

Cooperative Rotation and Spin Switching of Molecules in Artificial Arrays — •Niklas Ide, Arnab Banerjee, Richard Berndt, and Alexander Weismann — IEAP, Kiel, Germany

Artificial arrays of tin phthalocyanine (SnPc) molecules on Pb(100) substrate are investigated using a low-temperature scanning tunneling microscope. Switching the central SnPc molecule between its two out-of-plane configurations ($\mathrm{SnPc}\uparrow \rightarrow \mathrm{SnPc}\downarrow$) triggers a collective rotation of all surrounding molecules in the array. This correlated structural response is accompanied by a change of the molecular spin states. A model of the intermolecular and molecular substrate interactions reproduces the experimental observations.

O 69.5 Wed 18:00 P2

Nonalternant Carbon Nanoribbon with 4-5-6-8 Topology via Indenofluorene Polymer Fusion — •Dong Han[1], Tim Naumann[1], Faming Kang[1], Alexandr Oshchepkov[2], Mikhail Kalinin[2], Ye Liu[1], Zilin Ruan[1], Konstantin Y. Amsharov[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Organische Chemie, 06120 Halle (Saale), Germany

Carbon nanoribbons (CNRs) with nonhexagonal rings constitute a fascinating class of low-dimensional carbon materials exhibiting tunable chemical and physical properties distinct from those of conventional graphene nanoribbons (GNRs). Here, we report the on-surface synthesis and characterization of a nonalternant 4-5-6-8 CNR. This nanoribbon is obtained via lateral fusion of cis-linked indeno[2,1-a]fluorene (IF) polymer chains, formed by sequential debrominative and dehydrogenative C-C coupling reactions of a halogenated arene. Bond-resolved scanning tunneling microscopy (BR-STM) confirms the atomic structure of the resulting CNR. Scanning tunneling spectroscopy (STS) and density functional theory (DFT) calculations reveal its distinct electronic properties arising from the nonhexagonal rings. Notably, the 4-5-6-8 CNR exhibits a bandgap of 1.13 eV, highlighting the critical role of ring topology in modulating quantum confinement. X-ray photoelectron spectroscopy (XPS) further elucidates reaction pathways and intermediate species. This study establishes a controlled on-surface synthetic route towards structurally complex CNRs.

O 69.6 Wed 18:00 P2

Tuning electronic properties in 2D Covalent Organic Frameworks via on-surface chemistry — •Mira Sophie Arndt[1], Christoph Wachter[2], Roman Pallach[3], Yan Yan Grisan Qiu[4], Simone Mearini[4], Vitaliy Feyer[4], Sebastian Henke[3], Oliver T. Hofmann[2], Mirko Cinchetti[1], and Giovanni Zamborlini[5] — [1]Departement of Physics, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Department of Chemistry, TU Dortmund, Otto-Hahn-Straße 6, 44227 Dortmund, Germany — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [5]Institute of Physics, NAWI Graz, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Two-dimensional covalent organic frameworks (2D COFs) arranging in a Kagome lattice exhibit intriguing electronic properties, like flat bands and Dirac cones. We investigate the carbonyl-bridged aza-triangulene ($\mathrm{P^2}$TANGO), which assembles into a Kagome lattice on Au(111). Inspired by reports that deoxygenation of the precursor induces an open-shell triplet ground state, we explore hydrogen-assisted deoxygenation to tune the COF's electronic properties. Our angle-resolved photoemission measurements reveal changes in the electronic structure upon oxygen removal, including energy shifts of the dispersive valence band features. DFT confirms that the shift grows with the deoxygenation, and that, in case of a complete deoxygenation, the degeneracy between the flat bands and the Dirac-dispersing bands is lifted.

O 69.7 Wed 18:00 P2

On-surface Synthesis of Aza-Coronoids — •Tim Naumann[1], Zilin Ruan[1], Olaf A. Kleykamp[1], Linus Pohl[2], Anton Nizovtsev[2,3,4], Alix Kaczmarek[2], Eugen Sharikow[1], Jörg Sundermeyer[1], Doreen Mollenhauer[2,3,4], and J. Michael Gottfried[1] — [1]Marburg University, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [3]Helmholtz Institute for Polymers in Energy Applications Jena, Lessingstr. 12-14, 07743 Jena, Germany — [4]Institute for Technical and Environmental Chemistry, Friedrich-Schiller-Universität Jena, Philosophenweg 7a, 07743 Jena, Germany

Chemical reactivity and electronic properties of nanographenes are tailored by functionalization, edge topology and doping. A versatile subclass within the nanographenes are coronoids, defined as benzenoids featuring a cavity. π-extended coronoids possess low solubility and are challenging target molecules for in-solution chemistry. However, reliable access via on-surface synthesis was demonstrated. Here, we combined in-solution and on-surface techniques to gain access to various aza-coronoids. Besides planar armchair-edge and zigzag-edge terminated coronoids, a curved coronoid was synthesized. Nitrogen functionalization of the inner cavity allows for hosting a metal atom and yields coronoid-metal complexes. In contrast, nitrogen core-doping significantly alters the electronic properties. Low-temperature scanning tunneling microscopy/spectroscopy (STM/STS), non-contact atomic force microscopy (nc-AFM) and DFT calculations were performed.

O 69.8 Wed 18:00 P2

Bottom-up fabrication of molecular islands utilizing an SPM-based manipulation approach — •Mong-Wen Gu[1,2], Ruslan Temirov[1,2,3], F. Stefan Tautz[1,2,4], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [4]Institut für Experimentalphysik IV A, RWTH Aachen, Aachen, Germany

The scanning probe microscope (SPM) allows single molecules to be manipulated with very high precision. SPM-based manipulation provides an opportunity for the fabrication of nanostructures through bottom-up construction. One critical challenge is using molecules other than conventional CO molecules as building blocks. Here, we explore the parameter space of the manipulation process in which a single PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule bridges the SPM junction. We demonstrate the bottom-up construction of artificial PTCDA islands on Ag(111). These islands reproduce the native monolayer lattice structure, can be customized in size and shape and thus allow studying their electronic properties in a systematic way.

O 69.9 Wed 18:00 P2

Effect of the catalytic-substrate and graphene-films on the growth and physical properties of non-stoichiometric silicon-oxide nanoparticles — •Mehmet Selim Imamoglu, Cem Kincal, and Oguzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

It is well known that silicon-oxide particles form during the growth of graphene by chemical vapor deposition (CVD) in a quartz furnace. Our studies showed that the creation and structure of these particles is mostly governed by the hydrogen flow rate during growth. Moreover, we have proven that they can be covered by graphene films depending on their morphology; showing that graphene growth during CVD process can continue over a non-catalytic substrate. In this work we have further investigated the formation and physical properties of such nanoparticles. Our results indicated that CVD grown silicon-oxide nanoparticles have non-stoichiometric nature leading to photoluminescent behavior. In this presentation their structure and physical properties as a function of the growth substrate (Ni and Cu foils) and the existence or in-existence of graphene films will be discussed. We will also present the methodology to transfer these nanoparticles on to random substrates.

O 69.10 Wed 18:00 P2

Towards on-surface synthesis of helicene chains — •Jung-Ching Liu[1], Miguel Gavara[1], Kévin Martin[2], Narcis Avarvari[2], Karl-Heinz Ernst[3,4,5], and Johannes Barth[1] — [1]Department of Physics, Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany — [2]University of Angers, CNRS, MOLTECH-Anjou, SFR MATRIX, 49000 Angers, France — [3]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [4]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague 6, Czech Republic — [5]Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zürich, Switzerland

Helicenes are polycyclic aromatic helical compounds which have been investigated at surfaces regarding their spin selectivity due to their chirality and potential use in organic spintronics. To enhance chirality-induced spin selectivity, extended helicene chains are of interest. However, fabrication of such helicene chains has not yet been reported. Here, we present atomically precise dibromohexahelicene chain formations on Au(111). Investigated by STM and bond-resolving nc-AFM at 4K, we found self-assembled supramolecular clusters at low coverage. Coupling reactions occur as the annealing temperature reaches 330C. By further annealing to 380C, short segments of planar structures are found along with 3D chains. The findings indicate potential nanographenes formation, tentatively ascribed to a Diels-Alder pathway. Our study provides insights into extended on-surface synthesis using non-planar molecular precursors.

O 69.11 Wed 18:00 P2

Orthogonally oriented molecular motors assembled on the surface: from liquid-solid to ultrahigh vacuum — •Robby Reynaerts[1], Cosima Stähler[2], Steven De Feyter[3], Ben L. Feringa[2], and Leonhard Grill[1] — [1]Department of Chemistry, Division of Physical and Theoretical Chemistry, University of Graz, Heinrichstraße 28, 8010 Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, 9747 AG Groningen, The Netherlands — [3]Department of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

Molecular motors continue to attract wide interest, due to their capability to convert energy into uni-directional rotary motion at the nanoscale. Immobilization of molecular motors on a solid surface through molecular self-assembly could amplify their nanoscale motion. Applying specific molecular design such controlled assembly of molecular motors was achieved at the liquid-solid (LS) interface under ambient conditions and studied using scanning tunnelling microscopy (STM). However, the dynamics inherent to ambient conditions were inseparable from the response of the molecular motors to external stimuli. Bringing the system over to low temperature and ultra-high vacuum (LT-UHV) conditions would rid any inherent dynamics from those ambient conditions. In this contribution I will discuss the controlled self-assembly of molecular motors on a solid surface achieved through molecular design under ambient and LT-UHV conditions and the experimental transition between these conditions. References: Chem. Rev. 2005, 105, 1281; Chem. Eur. J. 2024, e202303994.

O 69.12 Wed 18:00 P2

Manipulation of Atomically Precise Nanostructures from Single Atoms and Molecules — •Nikita Osipov, Christophe Nacci, Grant J. Simpson, and Leonhard Grill — Physical Chemistry Department, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Quantum corrals are of particular interest in surface science as they can be used to investigate quantum phenomena, such as quantum mirage [1] or function as quantum simulators that mirror the electronic properties of real atoms or molecules [2]. Currently, investigating these prominent structures requires researchers to manually assemble the objects on a surface using atomic manipulation techniques, a process that is extremely time-consuming. Our work aims to solve this critical bottleneck and save valuable research time. A primary goal of our project is to create an instrument for automatic and autonomous atomic manipulation. We are developing this system using machine learning algorithms to enable the careful, precise positioning of atoms or molecules [3]. This novel instrument will facilitate the assembly of large-scale objects or complex compositions of multiple smaller ones with high precision, thereby enabling the collection of significantly more data. In this work, we present our current status of assembled quantum corrals on noble metal surfaces. First results of manually assembled nanostructures will be presented together with the computational algorithm in the automated construction. [1] Li, Q. et al., Nat. Commun. 11 (2020) 1400. [2] E. Sierda et al., Science 380 (2023) 1048-1052. [3] B. Ramsauer et al., J. Phys. Chem. A 127 (2023) 2041.

O 69.13 Wed 18:00 P2

Atomic-Scale Sequencing of Biomolecules with nc-AFM — •Benjamin Mallada[1], Alejandro Lynch-Gonzalez[1], Marko Grabarics[1], Pavel Jelinek[2], Bruno de la Torre[3], and Stephan

Rauschenbach[1] — [1]Department of Chemistry, University of Oxford, Oxford, UK — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]Nanomaterials and Nanotechnology Research Center (CINN-CSIC) , Mieres, Spain

Glycans, peptides, and cyclodextrins present major challenges for structural analysis due to branching, heterogeneous modifications, and stereochemical diversity. Conventional tools such as MS and NMR often fail to resolve these features at the single-molecule level. Noncontact AFM, combined with STM and KPFM under cryogenic UHV conditions, has recently demonstrated chemical sensitivity sufficient to discriminate functional groups and stereochemical arrangements by probing electrostatic and non-covalent interactions. Applications include the direct visualization of glycans in protein and lipid conjugates [1], submolecular resolution of cyclodextrins [2], and progress toward sequencing of complex carbohydrates and peptides. These results underline the potential of nc-AFM to expand the scope of SPM from imaging and identification toward true atomic-scale sequencing of biomolecules.