O 51: Focus Session: Molecular Nanostructures on Surfaces: On-Surface Synthesis and Single-Molecule Manipulation II

Time: Wednesday 15:00–17:45 Location: HE 101

Topical Talk O 51.1 Wed 15:00 HE 101

Exploring the Magnetic and Topological Properties in Carbon-based Nanomaterials — •Ping Yu — School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China

In low-dimensional carbon-based nanomaterials, quantum magnetism can be generated from the pi electrons, which have attracted lots of attention in the fields of on-surface synthesis and quantum spintronic materials. The talk will report on how to realize graphene-based quantum materials with desired magnetic or topological properties through on-surface synthesis. The electronic properties of designed graphene nanomaterials are comprehensively investigated by scanning probe microscope techniques and theoretical calculations. The results provide new strategies for designing and synthesizing nanographene materials with desired electronic functionalities.

O 51.2 Wed 15:30 HE 101

Polyradical State of an Extended Aza-Triangulene — •Francisco Romero-Lara[1], Alessio Vegliante[1], Manuel Vilas-Varela[2], Hector Briongos[1], Niklas Friedrich[1], Dongfei Wang[1], Ricardo Ortiz[3], Patrick Calupitan[3], Fabian Schulz[1], Thomas Frederiksen[3], Diego Peña[2], and Jose Ignacio Pascual[1] — [1]CIC nanoGUNE, Donostia, Spain — [2]CiQUS, Santiago de Compostela, Spain — [3]DIPC, Donostia, Spain

Triangulene nanographenes are the most paradigmatic case for the emergence of spin states due to the frustration of the bipartite lattice of graphene. Increasing their size implies an increase in sublattice imbalance, resulting in a larger spin state according to Lieb's theorem. Another way of controlling the spin state is by heteroatom substitution, e.g. N reduces the spin state by 1/2. In this work, we show that, by increasing the size of an aza-[3]-triangulene but maintaining the sublattice imbalance, the interplay between electron correlations and wavefunction hybridization is modified, resulting in a polyradical state. The successful synthesis of this extended triangulene on a Au(111) surface is confirmed by STM and nc-AFM with CO tips. We use STS to prove the magnetic character of the nanographene by measurements of the Kondo effect and spin excitations. Temperature and magnetic field dependence of the Kondo resonance indicates an $S=1/2$ ground state. Simultaneously, a spin excitation to a $S=3/2$ excited state was observed. These findings support the presence of a polyradical state in this nanographene conformed by three antiferromagnetically aligned radicals, in agreement with multireference CAS theoretical methods.

O 51.3 Wed 15:45 HE 101

Tuning the spin coupling in all-organic diradicals through mechanical manipulation — •Alessio Vegliante[1], Saleta Fernandez[2], Manuel Vilas-Varela[2], Ricardo Ortiz[3], Thomas Baum[4], Niklas Friedrich[1], Francisco R. Lara[1], Herre van der Zant[4], Thomas Frederiksen[3], Diego Peña[2], and Jose Ignacio Pascual[1] — [1]CIC NanoGUNE, Spain — [2]CiQUS-USC, Spain — [3]DIPC, Spain — [4]TU Delft, the Netherlands

Open-shell organic molecules have emerged as promising candidates for carbon-based spintronics. Organic diradicals, in particular, are interesting model systems for studying and manipulating intramolecular spin interactions at the atomic scale.

Here we report the tunable spin interactions of the molecular diradical 2OS on a Au(111) substrate using scanning tunneling microscopy and spectroscopy. 2OS is stable diradical, derivative of the Chichibabin*s hydrocarbon, characterized by a non-planar and flexible structure. With the support of theoretical calculations, we show that the spin interaction strongly depends on the structural conformation of the molecule: the adsorption on the Au surface induces a partial planarization that stabilizes a singlet ground state, while less planar conformations exhibit a significantly reduced spin coupling.

In this work, we demonstrate the possibility of tailoring the spin interaction through structural changes induced by approaching the STM tip or lifting the molecule from the substrate, thus confirming the influence of geometry on the molecule*s spin state.

O 51.4 Wed 16:00 HE 101

Charge states and electron correlation in graphene nanoribbons on MgO — •Leonard Edens[1], Amelia Domínguez Celorrio[2], Manuel Vilas-Varela[3], Sofia Sanz[4], Thomas Frederikssen[4], Diego Peña[3], Nacho Pascual[1], and David Serrate[2] — [1]CIC nanoGUNE, Spain — [2]CSIC-INMA and Universidad de Zaragoza, Spain — [3]CiQUS and Universidade de Santiago de Compostela, Spain — [4]DIPC, Spain

On-surface synthesis of graphene nanostructures provides tailor-made systems exhibiting quantum properties such as π magnetism. However, the underlying catalyst metal readily hybridizes with molecular orbitals and quenches spin. Here, we report the successful lateral STM manipulation of individual graphene nanoribbons onto epitaxial layers of MgO(001) after synthesis on Ag(001). We observe a rich electronic spectrum of large absolute gaps straddled by remarkably sharp resonances implying drastic lifetime enhancement. LDOS mapping allows exact determination of the large integer negative charge acquired due to the low insulator work function. We find that the integer charge state of the molecule depends on its length, leading to an opening and closing of the correlation gap with charge parity. Studying charge as a function of length shows that the electronic state alternates between open- and closed-shell as determined by the interplay between level evolution with length and electron correlation. We introduce a mean-field Hubbard model in the grand canonical ensemble that reproduces and predicts the charging behaviour and allows us to extract the energy of the graphene-metal interface dipole across the insulator.

O 51.5 Wed 16:15 HE 101

On-surface synthesis of non-planar carbon nanoribbons — Feifei Xiang[1], Sven Maisel[2], •Shreya Garg[1], Andreas Görling[2], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Graphene nanoribbons have great potential for applications in nanoelectronic devices such as transistors by combining the outstanding electronic properties of graphene with the introduction of an electronic band gap. In this study, we present a bottom-up synthesis approach for covalently linked non-planar carbon nanoribbons. We discuss the electronic properties of the non-planar carbon ribbons in relation to their adsorption geometry using low-temperature scanning tunneling microscopy and spectroscopy in combination with density functional theory. The synthesis involves bowl-shaped dibrominated indacenopicene precursors to create non-planar carbon ribbons through surface-assisted Ullmann-type dehalogenative coupling and cyclodehydrogenation on Au(111).

O 51.6 Wed 16:30 HE 101

Unipolar Resonant Hole Transport Through a Free-Standing Designer Graphene Nanoribbon — •Niklas Friedrich[1], Jingcheng Li[1], Iago Pozo[2], Diego Peña[2], and Nacho Pascual[1] — [1]CIC nanoGune, Spain — [2]CiQUS, Spain

Coherent electron transport through individual molecules is a vital technique to probe different quantum mechanical properties like energy level alignment, vibronic modes or spin states. Here, we investigate the electronic transport through 7-armchair graphene nanoribbons (GNRs) containing a single, substitutionally embedded 2B-dimer.

We find that the coherent electron transport through the 2B-GNR is unipolar with a singly occupied 2B-state (O2B) enabling resonant electron tunneling at both voltage polarities. The unipolar transport is favored by an exponential localization of the O2B resulting in a double tunneling barrier configuration. Further transport resonances reveal that resonant transport through the valence band exhibits a unipolar character, too. We find fingerprints of vibronic satellites and of band quantization in form of Fabry-Perot quantum well modes in our experiments.

The experiments were performed by lifting single 2B-GNRs using the tip of a low-temperature scanning tunneling microscope (STM) to create the molecular wires that bridges tip and substrate. Our results unravel the details of coherent resonant electron tunneling through molecular wires built from single 2B-doped GNRs, confirming their technological potential for single molecule electronics.

O 51.7 Wed 16:45 HE 101

On-Surface Synthesis of Edge-Extended Zigzag Graphene Nanoribbons — •Amogh Kinikar[1], Feifei Xiang[1], Xiushang Xu[2], Yanwei Gu[3], Akimitsu Narita[2], Klaus Müllen[2], Carlo Pignedoli[1], Oliver Gröning[1], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa, Dübendorf 8600 Switzerland — [2]OIST Graduate University, Okinawa 904-0495, Japan — [3]MPI-P, 55128 Mainz, Germany

Graphene nanoribbons (GNRs) have gained significant attention in nanoelectronics due to their potential for precise tuning of electronic properties through variations in edge structure and ribbon width. However, the synthesis of GNRs with highly sought-after zigzag edges (ZGNRs) remains challenging. Here, we present a design motif for synthesizing novel edge-extended ZGNRs. This motif enables the controlled incorporation of edge extensions along the zigzag edges at regular intervals, opening up possibilities for synthesizing a diverse range of edge-extended ZGNRs. Examples of successfully synthesized structures are presented, characterized using Scanning Tunneling Microscopy, and complemented by Density Functional Theory calculations. These efforts elucidate the electronic and magnetic properties of these edge-extended ZGNRs. The diverse range of edge-extended ZGNRs now possible expands the structural landscape of GNRs and facilitates the exploration of their structure-dependent electronic properties.

[1] Kinikar, A. et al. "On-surface Synthesis of Edge-Extended Zigzag Graphene Nanoribbons." *Advanced Materials* (2023) **35**, 2306311.

O 51.8 Wed 17:00 HE 101

How conductive is a single polyene chain? — •Sifan You[1], Yixuan Gao[2], Shixuan Du[2], and Lifeng Chi[1] — [1]Soochow University, Suzhou, China. — [2]Institute of Physics, Beijing, China

Conjugated polymers are promising candidates for molecular wires in nanoelectronics, with flexibility in mechanics, stability in chemistry and variety in electrical conductivity. Polyene, as a segment of polyacetylene, is a typical conjugated polymer with straightforward structure and wide-range adjustable conductance. To obtain atomic scale understanding of charge transfer in polyene, we measured the conductance of a single polyene-based molecular chain via lifting it up with scanning tunneling microscopy tip. Different from semiconducting characters in pristine polyene (polyacetylene), high conductance and low decay constant were obtained, along with an electronic state around Fermi level and characteristic vibrational mode.

O 51.9 Wed 17:15 HE 101

A Challenge Human vs Machine: Building a Nanopattern of Unknown Adsorbates — •Bernhard Ramsauer[1], Grant Simpson[1], Johannes J. Cartus[1], Leonhard Grill[2], and Oliver T. Hofmann[2] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, 8010, Austria — [2]Department of Physical Chemistry, Institute of Chemistry, NAWI Graz, University Graz, Graz, 8010, Austria

Scanning probe microscopes give us the possibility to precisely control the position and orientation of single molecules, thus unlocking the possibility to fabricate quantum-structures with novel properties. However, interaction processes at the nanoscale are stochastic, and the motion of molecules is often unintuitive and hard to predict even for human experts.

In this work we present an artificial intelligence challenging a human expert to build a pattern of unknown molecules as fast as possible. The challengers had one week each to learn the optimal manipulation parameters and to build the pre-defined nanopattern. In the building process every type of manipulation is allowed. Within this week one can attempt building the nanopattern as often as possible but the winner is determined by the shortest assembly time.

O 51.10 Wed 17:30 HE 101

Friction over single chemical bonds — Oliver Gretz[1], Lukas Hörmann[2,3], •Shinjae Nam[1], Oliver T. Hofmann[2], Franz J. Giessibl[1], and Alfred J. Weymouth[1] — [1]Universität Regensburg, Deutschland — [2]TU Graz, Österreich — [3]University of Warwick, UK

Friction is a phenomenon that acts on many different length scales. With a sharp nanometer-sized tip, lateral forces can be measured and phenomena like anisotropy or superlubricity can be observed [1, 2]. However, the *large* tip prevents measurements of single chemical bonds. But is this spatial resolution necessary to understand sliding friction? How much does the energy loss differ when sliding over different chemical bonds? We performed lateral force microscopy, in which the tip oscillates laterally above the surface, with small amplitudes and a CO-terminated tip to be directly sensitive to the dissipated energy above single chemical bonds [3]. By comparing the dissipation over different covalent bonds, we found that the local potential energy landscape plays an important role in sliding friction. We were also able to observe dissipation over single O**H bonds. Our findings show that a complete understanding of friction requires a description of the individual chemical bonds at the surface.

1.*Liley, M. et al., Science, 280(5361), 273-275, (1998). 2.*Dienwiebel, M. et al., Physical review letters, 92(12), 126101, (2004). 3.*Weymouth, A. J. et al., Physical Review Letters, 124(19), 196101, (2020).