O 69: Nanostructures at surfaces: 1D and 2D structures and networks II

Time: Wednesday 15:00–16:30 Location: MA 141

O 69.1 Wed 15:00 MA 141

Graphene nanoribbons on gold: superlubricity and edge effects — •Lorenzo Gigli — SISSA (International School of Advanced Studies), Via Bonomea 265, Trieste (TS), Italy

Via numerical simulations, we investigate the static structural features and the frictional response of n = 7 armchair graphene nanoribbons (GNRs) of different lengths deposited on a gold Au(111) substrate, a tribological interface subject of recent, intense experimental studies. The C-Au lattice mismatch and the GNR-substrate relative orientation dictate the periodicity of the interface Moire' pattern for the relaxed GNR configurations. By adiabatically increasing an uniform external force directed along the longitudinal GNR axis, the molecular-dynamics approach shows a static frictional response which does not grow with the GNR length, thus supporting the experimental data of a superlubric behavior with negligible frictional contribution of the internal bulk region of the ribbon. The peculiar oscillatory trend of the static friction versus length, around a fairly constant mean value (tens of pN), correlates with the characteristic modulation of the observed Moire' pattern (2D Materials 4, 045003, 2017).

Mimicking the experimental framework by Kawai et al. (Science 351, 957, 2016), we also present results of the dynamical response of deposited GNRs, lifted at one end and pulled laterally by a spring moving at constant velocity. Competition between peeling and sliding mechanisms, stick-slip and smooth dynamics are discussed in terms of the edge-lifting height and the effective GNR elasticity.

O 69.2 Wed 15:15 MA 141

Reaction pathway towards 7-armchair GNR formation and identification of intermediate species on Au(111) — Sebastian Thussing, •Sebastian Flade, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The reaction pathway of 10,10'-dibromo-9,9'-bianthryl (DBBA) deposited onto Au(111), eventually leading to the formation of 7-armchair graphene nanoribbons (7-AGNR) has been investigated. Individual reaction steps, along with the respective reaction intermediates were identified using IR-absorption and thermal desorption spectroscopy. They are characterized by distinct molecular species which have undergone (i) halogen abstraction, (ii) polymerization of the bianthryl units, (iii) H-abstraction and 5^+-AGNR formation, and (iv) further H-abstraction and 7-AGNR formation. Identification of surface species is aided by calculations of the vibrational properties of various model compounds. Comparison of TDS and IRAS data allows us to establish a correlation between individual surface reaction steps and processes leading to the desorption of molecular species, e.g. of intact DBBA, HBr, and H_2. Our refined model fully corroborates earlier observations of intermediate stages in the 7-AGNR formation using STM [1, 2].

[1] J. Cai et al., Nature 466 (2010) 470. [2] S. Blankenburg et al., ACS Nano 6 (2012) 2020.

O 69.3 Wed 15:30 MA 141

Magnetism in narrow graphene ribbons: open shells and quantum fluctuations — •Richard Korytár — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Graphene-type carbon structures are very frequently discussed for spintronics applications. These structures can host intriguing physical phenomena, such as electronic zero modes and localized spin states, with high relevance for the transport of spin and charge. I address some of these features in a prototypical example, the linear oligoacenes, which are the narrowest zig-zag graphene flakes. The importance of electron-electron interactions can not be underestimated as it underlies the effects such as edge-states or poly-radicals. I will examine the role of interactions by constructing an acene-like Hubbard model. The physics of non-interacting electrons manifests by peculiar oscillations of the excitation gaps with molecular length. The role of electron-electron interactions will be explored by comparing two approaches: an unrestricted Hartree-Fock and a numerically exact DMRG solution. Quantum fluctuations wipe out spin-polarized states and restore the band-structure effects in a large portion of the parameter space.

Wang, S. and Talirz, L. and Pignedoli, C. A. and Feng, X. and Müllen, K. and Fasel, R. and Ruffieux, P. Nature Communications 7, 11507 (2016)

P. Schmitteckert, R. Thomale, R. Korytár and F. Evers, The Journal of Chemical Physics 146, 092320 (2017)

R. Korytár, D. Xenioti, P. Schmitteckert, M. Alouani, F. Evers, Nature Communications 5 5000 (2014)

O 69.4 Wed 15:45 MA 141

Polymer Adsorption on Individual Single-Wall Carbon Nanotubes — •Matthias Josef Kastner[1] and Tobias Hertel[1,2] — [1]Institut für Physikalische und Theoretische Chemie, Julius-Maximilians-Universität Würzburg, Germany — [2]Röntgen Center for Complex Material Systems, Julius-Maximilians-Universität Würzburg, Germany

Polyfluorene copolymers are frequently used for the chirality-specific isolation of individualized Single-Wall Carbon Nanotubes (SWNTs). The interaction of polymers such as PFO-BPy with the carbon nanotube surface thus plays a key role in providing the desired selectivity. The objective of this work is to better understand and study the adsorption of single polymer strands on the SWNT surface by fluorescence microscopy and spectroscopy.

In the approach presented here we are using individual SWNTs, freely suspended across micron-sized trenches of a patterned SiO2 substrate and immersed in organic solvent. The adsorption of PFO-BPy is here monitored using changes in the intensity and center wavelength of SWNT exciton photoluminescence from individual nanotubes as a very sensitive probe for changes at the SWNT-solvent interface. Understanding of such adsorption processes is expected to lead into new insights which can be used for the chemical design of new selective polymers.

O 69.5 Wed 16:00 MA 141

Dependence of the adsorption height of graphene-like adsorbates on their dimensionality — •Serguei Soubatch[1], Simon Weiss[1], Xiaosheng Yang[1], Arnulf Stein[2], David Gerbert[2], Christine Brülke[3], Roman Kremring[3], Sascha Feldmann[2], Alex Schenk[4], Marie Gille[5], Timo Heepenstrick[3], Ina Krieger[3], Francois Bocquet[1], Stefan Hecht[5], Moritz Sokolowski[3], Petra Tegeder[2], and Stefan Tautz[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany — [3]Universität Bonn, Bonn, Germany — [4]La Trobe University, La Trobe, Australia — [5]Humboldt-Universität zu Berlin, Berlin, Germany

We measured the adsorption height of various graphene nanoribbons on the Cu(111) and the Au(111) surfaces and hexagonal boron nitride (hBN) and graphene on the Cu(111) surface using the x-ray standing waves technique. On Au(111), the different types of nanoribbons studied in our work are found to be physisorbed, while on Cu(111) the adsorption height is noticeably reduced pointing at a significant contribution of chemical interactions. Comparing to π-conjugated molecules on the one hand and hBN and graphene on the other, we observe a strong dependence of the adsorption height on the dimensionality of the adsorbate. This shows that graphene-like carbon adsorbates interact with the metal substrate mainly via the electron density of the honeycomb lattice. Chemical interactions involving edge atoms play a minor role.

O 69.6 Wed 16:15 MA 141

Light assisted charge spreading and charge trapping in organic semiconductors needles supported by 2D materials — •Aleksandar Matković[1], Markus Kratzer[1], Jakob Genser[1], Daniel Lüftner[2], Peter Puschnig[2], Zhongrui Chen[3], Olivier Siri[3], Conrad Becker[3], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Franz Josef Strasse 18, 8700 Leoben Austria — [2]Institute of Physics, University of Graz, NAWI-Graz, Universitätsplatz 5. 8010 Graz, Austria — [3]Aix Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France

In this study we investigate the growth of an oligoacene derivate dihydrotetraazaheptacene (DHTA7), which - due to nitrogen containing groups - forms solids through H-bonding and dipolar interactions between neighboring molecules. As a result of H-bonding networks, the molecules form in-plane rows with subsequent layers exhibiting π-π stacking. Crystalline needles of DHTA7 were grown by hot wall epitaxy on the surfaces of graphene and hexagonal boron nitride, which

act as van der Waals electrodes and gate dielectrics. Using photo-assisted electrostatic force microscopy we demonstrate charge trapping and light-assisted charge spreading within the networks of DHTA7 needles. We found that in the dark these needles are not conductive, while visible light linearly polarized parallel to the long axis of the needles allows spreading of the charges across the network for tens of micrometers. Results indicate that - due to the inverse population created by the laser - charges that were trapped in the localized defects can spread through the bands of the organic semiconductor.