O 14: Poster Session I: Nanostructures at surfaces I

Time: Monday 10:30–12:30 Location: P

O 14.1 Mon 10:30 P

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747AG Groningen, the Netherlands — [2]Strating Institute for Chemistry, University of Groningen, 9747AG Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material due to their excellent and tunable electronic properties. For instance, GNRs with armchair edge possess a width-dependent band gap, whereas zigzag GNRs are expected to host spin-polarized edge states and be semimetallic [1]. Previously, narrow chevron-like GNRs, which host a combination of zigzag and armchair edge terminations, were fabricated on a Au(111) substrate from the prochiral precursor 6,12-dibromochrysene through a combination of Ullmann-type coupling and cyclodehydrogenation [2]. Depending on the number of monomer units the ribbons are made of, an even and an odd number lead to a mirror and a point symmetric ribbon. Using scanning tunneling spectroscopy we investigated the potential effect of this length dependent symmetry on the electronic properties. In addition, we observed that through a common coupling defect bends are formed in the ribbons. We characterized these bends using a combination of high-resolution scanning tunneling microscopy and spectroscopy. It turned out the bends are based on the formation of both a five- and six-membered ring and that their electronic properties are altered. [1] K. Nakada et al., Phys. Rev. B 54, 17954 (1996) [2] T.A. Pham et al., Small 13, 1603675 (2017)

O 14.2 Mon 10:30 P

Thermally vs. Light-Induced On-Surface Polymerization — •Christophe Nacci and Leonhard Grill — Department of Physical Chemistry, University of Graz, Austria

Covalent on-surface polymerization via Ullmann coupling is one of the preferred chemical reactions to produce novel, and potentially functional, structures in the two-dimensional confinement of a surface. The dissociation of specific substituents and the formation of new covalent bonds can be induced by using different external stimuli, for instance heat, light and inelastic electron scattering. While plenty of examples exist on the thermal control of the reaction, only very few studies have reported a photochemical approach to form polymers at single-crystal surfaces. We compare the reaction pathways of individual molecular species to one-dimensional polymers by driving the reaction of the same precursor on Au(111) either by heat or by illumination with UV light. The results obtained by low-temperature scanning tunneling microscopy under ultrahigh vacuum conditions show that both stimuli are successful to induce the desired reaction on the surface. However, very different polymer length distributions are found, which will be discussed in view of the experimental conditions. Interestingly, under UV illumination the molecular coverage changes across the surface as it increases at the position of laser spot on the sample.

O 14.3 Mon 10:30 P

Adsorption Geometry and Intramolecular Reactions of 9-bromo-10- (1,1':3',1"-terphenyl-5'-yl)anthracene on Au(111) and Cu(111) — •Alexander Ihle[1], Daniel Ebeling[1], Doreen Mollenhauer[2], Hermann A. Wegner[3], and Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Germany — [2]Institute of Physical Chemistry, Justus Liebig University Giessen, Germany — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

On-surface chemistry is a powerful tool for building covalent molecular structures such as chains or graphene nanoribbons [1, 2]. Such tailored materials are interesting for future applications since their optical and electronic properties are controllable via their structure [3]. Furthermore, their main component carbon is environmentally friendly and sustainable. In addition to the structure of the precursors, the chemical properties of the substrate direct the reaction pathway. Using low-temperature atomic force microscopy with CO-functionalized tips, we identify the precise adsorption geometry of the pristine molecules, intermediates, and reaction products after subsequent heating steps. While the pristine molecules show similar features on both surfaces and adsorb quasi-planar, the adsorption geometry of the intermediates differs after heating depending on the substrate material. We suspect that different molecule-substrate interactions lead to this observation.

[1] Grill, L. et al. Nature Nanotechnology 2, 687-691 (2007)
[2] Cai, J. et al. Nature 466, 470-473 (2010)
[3] Zhong, Q. et al. J. Am. Chem. Soc. 141, 7399-7406 (2019)

O 14.4 Mon 10:30 P

Kinetically controlled on-surface playground of nanostructure growth — •Aisha Ahsan[1], Fatemeh Mousavi Mousavi[1], Thomas Nijs[1], Sylwia Nowakowska[1], Olha Popova[1], Aneliia Wäckerlin[1], Jonas Björk[2], Lutz Gade[3], and Thomas Jung[1,4] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]Department of Physics, Chemistry and Biology, IFM, Linköping University, Linköping 581 83, Sweden — [3]Anorganisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany — [4]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Rare gases on metals serve as models for understanding mass transport and crystal growth of adsorbates on surfaces, while LT-STM studies enriched our knowledge how rare gases behave at atomic level. Deep insight has been gained into the diffusion mechanisms of van der Waals adsorbates on a complex energy landscape defined by an on-surface coordination network architecture. Using Xe as the model case, a complex re-distribution/re-nucleation and coarsening/growth phenomena has been investigated where the adsorbate can be evaporated/recaptured into/from *gas phases* or *lattice gas phases* between 5K and 50K showing hopping motion between different confinements (0D), along boundaries of network (1D) and across whole network backbone (2D). After heating to ~50K then back to 5K, atoms are exclusively found in the thermally minimal state of 12 Xe atoms filling one pore, a process which we assign to the analogon of Ostwald ripening/coarsening transition which clearly limited in size.

O 14.5 Mon 10:30 P

Electrospray Ion Beam Deposition of Biological Molecules — •Henrik Siboni[1,2], Andreas Zimmer[2], and Leonhard Grill[1] — [1]Single-Molecule Chemistry, Institute of Chemistry, University of Graz, Austria — [2]Pharmaceutical Technology & Biopharmacy, Institute of Pharmaceutical Sciences, University of Graz, Austria

Scanning Tunneling Microscopy under Ultra-High Vacuum (UHV) conditions is a powerful method to image single molecules. However, its application in biophysics and pharmacy is limited by the fact that thermal sublimation, which is the common deposition method under UHV, requires rather high temperatures, due to the large molecular mass and thus low vapour pressures. This typically leads to molecular fragmentation before they can adsorb on a surface. Drop casting, on the other hand, can leave too much solvent contamination. In this poster, electrospray ion beam deposition of biological molecules will be presented where the molecules are gently transferred from solution under atmospheric pressure to a single-crystal metal surface at UHV pressure.

O 14.6 Mon 10:30 P

Defect-mediated *ab initio* thermodynamics of metastable γ-MoN(001) — •Giyeok Lee[1], Hojun Lee[1], Taehun Lee[1,2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Chemistry, Princeton University, Princeton, New Jersey 08540, United States

Refractory transition metal nitrides exhibit a plethora of polymorphic expressions and chemical stoichiometries. To afford a better understanding of how defects may play a role in the structural and thermodynamics of these nitrides, using density-functional theory calculations, we investigate the influence of point and pair defects in bulk metastable γ-MoN and its (001) surface. We report favorable formation of Schottky defect pairs of neighboring Mo and N vacancies in bulk γ-MoN and apply this as a defect-mediated energy correction term to the surface energy of γ-MoN(001) within the *ab initio* atomistic thermodynamics approach. We also inspect the structural distortions in both bulk and surfaces of γ-MoN by using the partial radial distribution function, $g(r)$ of Mo-N bond lengths. Large atomic displacements are found in both cases, leading to a broad spread of Mo-N bond length values when compared to their idealized bulk values. We propose that these structural and thermodynamic analysis may provide some insight to a better understanding of metastable materials and their surfaces.

O 14.7 Mon 10:30 P

Completing the Picture of Embryonic Oxidation on Copper — •Yun-Jae Lee[1], Trinh Thi Ly[2], Taehun Lee[1], Krisztián Palotás[3], Se Young Jeong[4], Jungdae Kim[2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering and Center for Artificial Synesthesia Materials Discovery, Yonsei University, Seoul 03722, Republic of Korea — [2]Department of Physics, and EHSRC, University of Ulsan, Ulsan 44610, Republic of Korea — [3]Institute for Solid State Physics and Optics, Wigner Research Center for Physics, 1525 Budapest, Hungary — [4]Department of Optics and Mechatronics Engineering, Pusan National University, Busan 46241, Republic of Korea

The oxidation of copper surfaces has been studied extensively in the literature – from simple oxygen chemisorption to the formation of complex surface oxides. Having an accurate atomistic model for this metal/oxide interface plays a pivotal role in determining interfacial processes in many copper-based technologies. The “29” and “44” complex surface oxides represent two of the most classical embryonic oxides on Cu(111). Although many attempts have been made to offer a detailed atomistic model of these surface oxides, their atomic structures remain ambiguous. In this work, we address this open question via *ab initio* scanning tunneling microscopy simulations that go beyond the simplistic Tersoff-Hamann approach where the (functionalized) metal tips are explicitly included, and are corroborated by high-resolution STM experiments. In particular, we reexamine the “29” structure and elucidate a complete atomistic model for the “44” structure.

O 14.8 Mon 10:30 P

Nano-hillock formation on $\mathbf{CaF_2}$ due to individual slow Au-cluster impacts — •Gabriel L. Szabo[1], Markus Lehner[1], Lothar Bischoff[2], Wolfgang Pilz[2], Ulrich Kentsch[2], Friedrich Aumayr[1], Nico Klingner[2], and Richard A. Wilhelm[1] — [1]TU Wien, Institute of Applied Physics, 1040 Vienna, Austria — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Ion-irradiation of surfaces was found to be a very powerful technique for surface modifications on a large amount of technologically relevant materials. Especially the formation of nanostructures, such as iontracks and nano-hillocks, which are mediated by electronic excitation induced by slow highly charged ions and swift heavy ions received lots of interest in recent years. For those experiments, the ionic crystal CaF_2 was a model system for the underlying processes. We use the same model system here, but a more direct way of creating nanohillocks by heavy cluster irradiation. In our investigations we show the formation of nano-hillocks by slow individual Au-cluster-irradiation on $CaF_2(111)$ surface that are very similar to hillocks iobserved previously with highly charged ions. We show that the size of the hillocks can be tuned by the cluster size.

O 14.9 Mon 10:30 P

A molecular quantum ring formed from a π-conjugated macrocycle — Chris J. Judd[1], Anton S. Nizovtsev[2,3,4], Rikke Plougmann[1], Dmitry V. Kondratuk[5], Harry L. Anderson[5], Elena Besley[2], and •Alex Saywell[1] — [1]School of Physics & Astronomy, University of Nottingham, UK. — [2]School of Chemistry, University of Nottingham, UK. — [3]Nikolaev Institute of Inorganic Chemistry, Russian Academy of Sciences, Russian Federation. — [4]Novosibirsk State University, Russian Federation. — [5]Department of Chemistry, University of Oxford, UK.

Quantum rings are structures that facilitate phase-coherent electron motion around a closed path and exhibit quantum phenomena; e.g. persistent currents and the Aharonov-Bohm effect. Our approach utilises cyclic porphyrin polymers, possessing a delocalised π-conjugated electronic structure [1], as molecular quantum rings.

We present details from our recent work [2] where the electronic structure of a molecular quantum ring (a 40 unit cyclic porphyrin polymer within stacks of 2-3 rings supported on a Ag(111) substrate) is characterised via scanning tunnelling microscopy (STM) and scanning tunnelling spectroscopy (STS). Combining density functional theory and tight binding calculations, in concert with experimental data, we interpret the experimentally obtained electronic structure in terms of quantum states confined around the π-conjugated macrocycle.

[1]M.D. Peeks,et al., Nature 541, 200 (2017).[2]C.J. Judd, et al., Phys.Rev.Lett. 125, 206803 (2020).