O 71: Poster Wednesday: Adsorption and Catalysis

Time: Wednesday 17:45–20:00 Location: Poster B2

O 71.1 Wed 17:45 Poster B2

Synthesis on surfaces: direct desulfurization and hyperthermal reactions of Reichardt's dye — •Tomasz Michnowicz[1], Bogdana Borca[1,2], Rémi Pétuya[3], Marcel Pristl[1], Ulrike Kraft[1], Hagen Klauk[1], Pavel Jelinek[4], Andres Arnau[3], Uta Schlickum[1,5], Lukas Krumbein[1], Suman Sen[1], Martina Stella[6], Andrea Floris[6], Allesandro de'Vita[6], Stephan Rauschenbach[1,7], and Klaus Kern[1,8] — [1]Max Planck Institute for Solid State Research, Germany — [2]National Institute of Materials Physics, Romania — [3]UPV/EHU San Sebastian, Spain — [4]Insitute of Physics CAS, Czech Republic — [5]TU Braunschweig, Germany — [6]King's College, UK — [7]University of Oxford, UK — [8]École Polytechnique Fédérale de Lausanne, Switzerland

We present combined STM/AFM studies of molecular structures acquired via two different approaches to on-surface chemical reactions: local, precise control of a desulfurization process and a kinetically induced reaction of Reichardt's dye. The first reaction is driven by the local electric field present in the STM tip-sample junction. We demonstrate the subsequent dissociation of both carbon - sulfur bonds of a thiophene group embedded in tetracenothiophene (TCT) molecules on Cu(111). For the second system we utilize the Electrospray Ion Beam Deposition (ES-IBD) to collide single molecular ions of Reichahrdt's dye with a Cu(100) surface at energies in the hyperthermal regime. With this technique, new species of Reichhardt's dye can be obtained (e.g. including ruptured benzene rings), inaccessible by means of a standard thermal activation path.

O 71.2 Wed 17:45 Poster B2

Model catalytic studies of liquid organic hydrogen carriers: Indole/Indoline/Octahydroindole on Ni(111) — •Johann Steinhauer, Philipp Bachmann, Udo Bauer, Fabian Düll, Florian Späth, Hans-Peter Steinrück, and Christian Papp — Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

The availability of energy from renewable sources is unsteady and unpredictable due to environmental influences. Therefore, energy storage becomes more important in the near future. One route to store energy in the form of hydrogen are liquid organic hydrogen carriers (LOHCs) that enable chemical storage of hydrogen. In an LOHC system, organic molecules are catalytically loaded with hydrogen to form an energy- and hydrogen-rich compound. Afterwards, hydrogen is catalytically unloaded. Recent studies identified the N-based heteroalicyclic system N-ethylcarbazole (NEC) as suitable LOHC (hydrogen capacity of 5.8 wt%). Herein, we present detailed studies on the LOHC system indole, with the hydrogen-rich octahydroindole (hydrogen capacity of 6.4 wt%), the dehydrogenation intermediate indoline and the hydrogen-lean indole. This system is investigated in a model approach on a Ni(111) surface under ultra-high vacuum conditions. HR-XPS and TPD are used to provide insights in the adsorption, desorption and reaction behavior of the LOHC system. We will present a detailed description of the reaction pathway and discuss the use of this system for chemical hydrogen storage. A comparison and evaluation of the differences to the known system H12-NEC / NEC will be presented.

O 71.3 Wed 17:45 Poster B2

A confined hydrogen molecule chopping light emission from a tunnel junction — Pablo Merino[1,2,3], Anna Rosławska[1], Christopher C. Leon[1], Christoph Grosse[1], César González[4], •Klaus Kuhnke[1], and Klaus Kern[1,5] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Instituto de Ciencia de Materiales de Madrid, Spain — [3]Instituto de Física Fundamental, Madrid, Spain — [4]Departamento de Física Teorica de la Materia Condensada, Madrid, Spain — [5]École Polytechnique Fédérale de Lausanne, Switzerland

We combine scanning tunneling microscopy (STM) with optical correlation spectroscopy to access the dynamics of H_2/Au(111). At low coverage (ca. 2%) molecular hydrogen forms a hexagonal superlattice with a large intermolecular spacing of 2 nm ascribed to molecular interaction dominated by surface state electrons at the Fermi energy. We characterize this yet unexplored glassy phase which provides an open structure in which a single molecule is confined - yet free to move in and out of the tunnel junction. Plasmonic light emission from the STM junction in constant height mode is employed to observe this motion by means of the resulting intensity modulation. Analyzing the time-resolved photon train detected in the far-field provides an autocorrelation function $g^{(2)}(\Delta t)$ which is dominated by one exponential. The residence time in the junction (10 ms) and the out-of-junction excursion time (3 ms) are obtained by modeling the system with a two-state (in-junction ⇔ out-of-junction) rate equation model.

O 71.4 Wed 17:45 Poster B2

Moving atoms on surfaces: The impact of external parameters on the required force — Jonathan Brand, •Nicolas Néel, and Jörg Kröger — Technische Universität Ilmenau, Ilmenau, Germany

Combining scanning tunneling microscopy and atomic force spectroscopy the dependence of the lateral force to move single adsorbed atoms on surfaces on the temperature is explored. A decrease of the force with increasing temperature is observed for all atoms and surfaces investigated and may be captured in a simple model. Crossing the critical temperature as well as surmounting the critical magnetic field of a superconductor does not lead to discriminable changes in the lateral force.

O 71.5 Wed 17:45 Poster B2

Addressing individual redox states of single polyoxovanadate molecules — •Marco Moors[1], Oliver Linnenberg[2], and Kirill Yu. Monakhov[3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52425 Jülich — [2]Institut für Anorganische Chemie, RWTH Aachen, Landoltweg 1, 52074 Aachen — [3]Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, 04318 Leipzig

Polyoxometalates (POM) offer a great potential for future applications in the fields of catalysis, sensors or molecular data storage. An outstanding property of POM consisting of vanadium ions is the ability of the latter to transit between multiple stable redox states, without affecting the structural integrity of the molecule [1]. In this study we present a model approach for tailoring and testing tris(alkoxo)-terminated Lindqvist-type POM as operational units for (multi-)resistive switching memories. This POM class is characterized by a rather small negative molecular charge of its fully-oxidized species and can be easily derivatized with different organic ligands. By applying an external potential we were able to demonstrate the controlled addressing of individual redox states of a single molecule adsorbed on an Au(111) surface at room temperature [3].

[1] K. Y. Monakhov et al., Adv. Inorg. Chem. 69 (2017) 251; [2] D. Li et al., J. Am. Chem. Soc. 133 (2011) 14010; [3] O. Linnenberg et al., J. Am. Chem. Soc. DOI: 10.1021/jacs.8b08780 (2018).

O 71.6 Wed 17:45 Poster B2

Epiminotetracenes on Au(111) — •Frank Eisenhut[1,2], Dmitry Skidin[1,2], Fátima García[3], Diego Peña[3], Gianaurelio Cuniberti[1,2,4], and Francesca Moresco[1,2] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica, Universidade de Santiago de Compostela, 15782-Santiago de Compostela, Spain — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

The introduction of substituents into the aromatic core has been proven to be a versatile tool in the generation of acenes. Within this study, we use a tetracene precursor with two embedded epimino-groups in the aromatic backbone, wehreas after moderate annealing one nitrogen-carbon bond can be cleaved or the complete group can be dissociated. This partial reaction has been proven with high-resolution STM images. While we could verify that the originated tetracene molecules with two of these new formed groups are strongly bonded to the surface and cannot be manipulated, we could show that the molecules with one nitrogen-containing side group after the reaction can be rotated around the nitrogen atom. Consequently, the molecules are anchored on Au(111) with nitrogen-gold bonds via the emerging side groups after the planarization and breaking of the bond.

O 71.7 Wed 17:45 Poster B2

Anchoring strategies for a molecular gear on Au(111) — •Tim Kühne^{1,2}, Frank Eisenhut^{1,2}, Jorge Monsalve^{1,2}, Claire Kammerer^{3}, Gianaurelio Cuniberti^{1,2,4}, and Francesca Moresco^{1,2} — ^{1}Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — ^{2}Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — ^{3}CEMES, Université de Toulouse, CNRS, Toulouse, France — ^{4}Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

A fundamental component of a planar single-molecule mechanical machine is a molecular gear, whose construction needs a proper combination of the molecular design, a smart selected surface for anchoring as well as the controlled rotation by manipulation. We investigated the adsorption of single pentaphenylcyclopentadiene molecules (PPCP) on Au(111) by LT-STM. We took advantage of the radical character after the tip-induced dehydrogenation of the single hydrogen at the cyclopentadiene core and studied the step-by-step rotation of this species using the lateral manipulation mode. As a last approach, we positioned PPCP on gold atoms and -clusters to examine the usage of these clusters as gear wheel axles.

O 71.8 Wed 17:45 Poster B2

Hydrogenation of ethylene on supported size-selected Pt-clusters — •Kevin Bertrang, Maximilian Krause, Marian Rötzer, Andrew Crampton, and Ueli Heiz — Chair of Physical Chemistry, Department of Chemistry & Catalysis Research Center, Technische Universität München, Lichtenbergstraße 4, 85748 Garching, Germany

The interplay between catalyst and support, e.g. thin silica films on metal single crystals, has proven a key factor in the activity of such systems. The nature of their interaction determines the charge transfer to the supported catalyst and therefore its electronic proprieties. The catalyst's local electron density can be altered by varying the underlying metal, which allows to tune the reactivity of the catalyst by specifically (de)charging it. Additionally to the bonds formed at the metal-silica interface, the resulting local work function of the support was found to govern charging effects. A system exhibiting a high local work function yields cluster of positive partial charge, vice versa clusters are partially charged negative with a low local work function. In this context, the change in activity of size-selecteed Pt-clusters towards ethylene hydrogenation has been investigated under steady-state conditions supported on thin silica films on different metal single-crystals. The catalytic samples were characterized through TPD, IRRAS and electron spectroscopy.

O 71.9 Wed 17:45 Poster B2

Effect of molecular structures on Metathesis reaction and its potential application — •Xiangzhi Meng^{1,2}, Lacheng Liu^{1,2}, Fatima Garcia^{3}, Berta Alvarez^{3}, Dolores Perez^{3}, Hong-Ying Gao^{1,2}, Diego Pena^{3}, and Harald Fuchs^{1,2} — ^{1}PhysikalischesInstitut,WestfalischeWilhelms-UniversitaẗMünster,Wilhelm-Klemm-Straße10,48149Münster,Germany — ^{2}Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster, Germany — ^{3}CentrodeInvestigacioń enQuímicaBioloxicaeMateriais-Moleculares(CIQUS)andDepartamentodeQuímicaOrgańica, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain

Recently, the σ-bond metathesis reaction has been reported between aromatic silylated alkynes and carboxylic acids on metal surfaces. Here, we further studied the effect of the molecular structures on the metathesis reaction on different (111) surfaces. Two silylated tetraynes with nonaromatic alkene and aromatic naphthalene as central cores were prepared and tested together with aromatic acids. A low-temperature scanning tunneling microscope was used. We found the aromatic tetrayne has a higher reactivity in the metathesis reaction than the nonaromatic tetrayne. It is also found that the metathesis reaction is surface-dependent. The metathesis reaction could become a new method for the bottom-up strategies and the related discoveries here will open new doors for the molecular designs in on-surface reactions.