

O 51: Poster Session - Metal Substrates: Adsorption and Reaction of Small Molecules

Time: Tuesday 18:15–20:00

Location: P2/10G

O 51.1 Tue 18:15 P2/10G

Electronic Structure of a Highly Ordered B₃N₃-Doped Nanographene Monolayer on Au(111) — ●AXEL BELSER¹, KATHARINA GREULICH¹, HOLGER F. BETTINGER², HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tuebingen — ²Institute of Organic Chemistry, University of Tuebingen

Electronic interface properties and the initial growth of hexa-*peri*-hexabenzocoronene with a borazine core (BN-HBC) on Au(111) have been studied by using X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). The results are compared to hexa-*peri*-benzocoronene (HBC). Both molecules form well-defined monolayers, in particular after annealing of 2-3 monolayers to 300 °C. Valuable information about the electronic structure is obtained by a variation of the tunneling voltage. The distribution of the HOMO and the LUMO determined tentatively by STM is in good agreement to DFT calculations.

O 51.2 Tue 18:15 P2/10G

probing water overlayer on Pt(111) by noncontact atomic force microscopy — ●SIFAN YOU¹, JING GUO^{1,2}, DUANYUN CAO¹, JI CHEN¹, XINZHENG LI¹, LIMEI XU^{1,3}, ENGE WANG^{1,3}, and YING JIANG^{1,3} — ¹School of Physics, Peking University, Beijing 100871, P. R. China — ²Beijing Normal University, Beijing 100875, P. R. China — ³Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

As a common and efficient catalyst in electrochemical reactions, platinum has attracted lots of attentions. Imaging the water structures at atomic level may help us to achieve a better understanding of electrical double layer near the electrode and active sites during the catalytic process. Using qPlus-based noncontact atomic force microscopy, here we were able to image partial dissociation of the first water overlayer on Pt(111) with unprecedented resolution. For the root square 37

structure, it is consistent with the previous results, showing a mixture of 5-6-7 water rings. Combined with X-ray photoelectron spectroscopy, we identify the structural evolvement of the water layer from intact *37**37 phase to a partially dissociated 3*3 phase after low-temperature annealing. Temperature and isotope dependent measurements clearly show that the transition involves a proton tunneling process, which is facilitated by a collective rearrangement of H-bonding network. This work reveals the key role of nuclear quantum effects in the surface-catalyzed water dissociation.

O 51.3 Tue 18:15 P2/10G

Fusion of alkyl groups to form phenyl rings: a new on-surface reaction — ●AMOGH KINIKAR¹, MARCO DI GIOVANNANTONIO¹, JOSÉ IGNACIO URGEL¹, KRISTJAN EIMRE¹, CARLO PIGNEDOLI¹, XIAO-YE WANG², ZIJIE QIU², AKIMITSU NARITA², KLAUS MÜLLEN², PASCAL RUFFIEUX¹, and ROMAN FASEL¹ — ¹Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, 8600, Switzerland — ²Max Planck Institute for Polymer Research, Mainz, 55128, Germany

On-surface synthesis allows for the design of carbon nanostructures such as graphene nanoribbons with atomic precision. However, the variety of conceivable structures critically depends on the number of available reactions. Here, we present a new surface-assisted reaction allowing for the controlled fusion of two alkyl groups to form a phenyl ring mediated by the activation of alkyl C-H bonds under ultra-high vacuum conditions. Scanning tunneling and non-contact atomic force microscopy images at different stages of the reaction along with DFT simulations allow us to elucidate the reaction mechanism. Furthermore, we study the influence of surface templating by comparing the reaction on Au(111) and Au(110). The selective formation of phenyl rings by the on-surface fusion of alkyl groups is unprecedented, and introduces a powerful new motif for the design of novel carbon nanomaterials while furthering our understanding of the reactive nature of the alkyl C-H bonds.