O 60: Post Deadline Session followed by Surface Science "get-together"

Time: Thursday 20:00–21:00 Location: HSZ 02

O 60.1 Thu 20:00 HSZ 02

Can molecular orbitals be simply reconstructed from photoemission data? — •Peter Puschnig[1], Claudia Ambrosch-Draxl[1], Thomas Seyller[2], Stephen Berkebile[3], Georg Koller[3], Falko P. Netzer[3], and Michael G. Ramsey[3] — [1]Chair for Atomistic Modelling and Design of Materials, University Leoben — [2]Institut für Technische Physik II, Universität Erlangen-Nürnberg — [3]Surface Science Group, Institute of Physics, University Graz

We present a new and simple approach with the aim to determine the shape of molecular orbitals by means of angle-resolved photoemission (PE) experiments. It applies to molecular films ranging from monolayers up to multilayers and leads to images of individual molecular states with a spatial resolution of about 1 Å, thereby competing with state-of-the-art scanning probe techniques. We demonstrate how the PE intensity recorded over a hemispherical region generates reciprocal space maps of the initial state. This data provides unambiguous fingerprints of individual molecular orbitals and is used to reconstruct real space images of the frontier molecular orbitals in good agreement with density functional (DFT) calculations. With k-space maps obtained using the toroidal analyser at BESSY II we demonstrate the viability of the proposed method even for the strongly bound monolayer of para-sexiphenyl adsorbed on Cu(110). Here the reconstructed HOMO and ex-LUMO orbital can both be clearly recognized and compare well to the DFT results. The generality of the approach is then illustrated with examples from molecular films ranging from the small rod-like pentacene to the plate-like tetraphenylporphyrin.

O 60.2 Thu 20:15 HSZ 02

Localization of Electronic States within a Moiré Pattern — •Thiruvancheril G. Gopakumar, Nicolas Néel, Jörg Kröger, and Richard Berndt — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Moiré patterns have been observed for various heteroepitaxial layers. Little is known about the electronic structure on a nanometre scale of these regular superlattices. We use a cryogenic scanning tunnelling microscope to probe the electronic properties of a moiré pattern observed from Co islands on Ag(111). Spatially resolved spectroscopy reveals that the moiré pattern gives rise to a striking localization of Co *d*-states. We use these states as an electronic template to guide the arrangement of magnetic molecules.

O 60.3 Thu 20:30 HSZ 02

Polar catastrophe and how thin $LaAlO_3$ films on $SrTiO_3$(001) deal with it — •Rossitza Pentcheva[1] and Warren E. Pickett[2] — [1]Dept. of Earth and Environmental Sciences, University of Munich — [2]Dept. of Physics, University of California at Davis

Even at the interface of conventional band insulators polar discontinuities can drive novel electronic behaviour: An example is the two-dimensional electron gas [1] and thickness dependent switching from insulating to conducting behaviour [2] reported in thin $LaAlO_3$ films on a $SrTiO_3$(001)-substrate.

Density functional theory calculations reveal that a strong polar distortion creates the necessary screening and enables several unit cells of $LaAlO_3$ to sustain their ionic charges and remain insulating. However, the band gap of the system, defined by O 2*p* states at the surface and Ti 3*d* states at the interface decreases with each added $LaAlO_3$-layer, before an insulator-to-metal transition and a crossover to an electronic reconstruction (as observed previously at the isolated interface [3]) takes place at around 5 monolayers of $LaAlO_3$. The implications of two different, spatially separated types of carriers - holes at the surface and electrons at the interface - will be discussed.

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[1] A.Ohtomo and H.Y.Hwang, Nature **427**, 423 (2004)
[2] S.Thiel *et al.*, Science **313**, 1942 (2006)
[3] R. Pentcheva and W.E. Pickett, Phys. Rev. B. **74**, 035112 (2006); ibid. **78**, 205106 (2008).

O 60.4 Thu 20:45 HSZ 02

Photo resist free patterning by local oxidation of Ag surfaces — •Sebastian Günther[1], Robert Reichelt[1], Joost Wintterlin[1], Andrea Locatelli[2], Miguel Niño[2], Tefvik Menteş[2], and Alexei Barinov[2] — [1]Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstr. 11, 81377 München, Germany — [2]Sincrotrone Trieste S.C.p.A., Area Science Park, 34012 Basovizza-Trieste, Italy

Traditional surface patterning processes usually make use of photo resists and require several preparation steps such as resist irradiation and development, etch or deposition steps and eventually lift off processes. Here, we report on a potential single step structuring process which can be used to chemically pattern Ag surface by a local oxidation reaction. In particular, we present our recent findings that low energy electron irradiation of Ag(111) or polycrystalline Ag during NO2 adsorption at 300 K induces the formation of Ag oxide. Using a spatially confined electron beam, small Ag2O spots could be grown with sharp, ˜ 100 nm wide, boundaries to the non irradiated metallic surface. The structure may be written as well by photon instead of electron irradiation, which makes the use of masks possible. Since the structure size will mainly depend on the sharpness of the irradiation electron beam or of the applied masks, the observed process has the potential of a single step nanostructuring process. Temperature treatment offers an easy way to manipulate the boundary between oxide and metallic silver by steering chemical fronts.