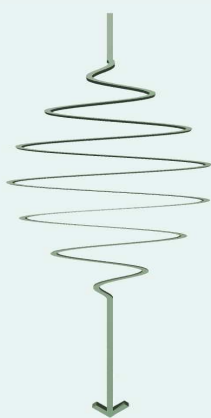


February 15th, 2012 - 15:00 pm

Seminar Room 108, DESY Bldg. 49



Max Planck
Research
Department
for
Structural
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SEMINAR

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Formation Mechanism of Metal-Organic Interface States studied by 2-Photon-Photoemission-Spectroscopy

For functional devices in organic electronics the charge carrier injection from the metal electrodes into the active organic regions to a large extent determines the device efficiency. These dynamical processes strongly depend among others on the energetic alignment of molecular states and the metallic Fermi level E_F as well as newly emerging interface states due to the chemical bonding or the modified symmetry at the interface. They can best be investigated by applying time- and angle-resolved 2-photon photoemission (2PPE) to study structurally well characterized organic thin films adsorbed on single crystal metal surfaces.

Interface states that are located between the Fermi level of the metal and the LUMO level of organic molecules are expected to have a decisive influence on the charge carrier injection across a metal-organic interface. Such an interface state was characterized recently for the interface between monolayer films of the organic semiconductor 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) and a Ag(111) surface [1]. The Shockley State maintains its metal character but is shifted in energy and forms an unoccupied strongly dispersing state with a short inelastic lifetime of 54 fs. In order to gain insight into the mechanisms that lead to the formation of such interface states and to understand their properties we have investigated 1,4,5,8-naphthalene tetracarboxylic acid diandrydride (NTCDA) which is strongly related to PTCDA but has a weaker interaction the Ag(111) substrate. The opposite case of a stronger bound molecular layer can be studied for the disordered low-temperature phase of PTCDA [2]. For both interfaces, we observe similar interface states that emerge from the Shockley-surface state due to the interaction of the first molecular layer with the Ag(111) substrate. By combining our 2PPE investigations on the different model systems with density functional theory calculations, we are able to extract the fundamental physical processes that determine the energetic position of these Shockley-derived interface states and their overlap with molecular states [3].

- [1] C. H. Schwalb et al., Phys. Rev. Lett. 101, 146801 (2008).
- [2] L. Kilian et al., Phys. Rev. Lett. 100, 136103 (2008)
- [3] M. Marks et al., Phys. Rev. B 84, 081301(R) (2011)



Host: Sebastian Loth, MPSD, CFEL