

Organic charge-transfer complexes on Ag(111)

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In recent years, molecular layers consisting of electron donating and accepting molecules have attracted increasing attention due to their potential usage in optoelectronic devices. Here we report on the formation of a blend of organic donors and acceptors from 1,4,5,8,9,12-hexaazatriphenylene-hexacarbonitrile (HATCN) and 2,3,6,7,10,11-hexakis-alkoxytriphenylene (HAT) on a Ag(111) surface^[1]. We used scanning tunneling microscopy and spectroscopy (STM/STS), ultraviolet and x-ray photoelectron spectroscopy (UPS/XPS), angle-resolved photoemission spectroscopy (ARPES) and low-energy electron diffraction (LEED) measurements complemented by density functional theory (DFT) calculations to investigate both the electronic and structural properties of the homomolecular as well as the intermixed molecular layers. Both molecules assembled on Ag(111) into well-ordered and commensurate structures at monolayer coverage. For a homomolecular layer of the electron donor HAT, we found a weak interaction with the Ag(111) surface, while for the electron acceptor HATCN a strong interaction with the substrate leading to charge transfer and substantial buckling of the top silver layer as well as of the adsorbates was determined. Upon mixing acceptor and donor molecules (ratio of 1:1), a strong hybridization between the two different molecules leading to the emergence of a common unoccupied molecular orbital located at both - donor and acceptor molecule - was found. In addition, our results suggest that the intermolecular interactions are strongly increased in the intermixed layer compared to the homomolecular ones, while especially the HATCN-substrate interaction is significantly reduced. The donor acceptor blend studied is therefore a compelling candidate for the fabrication of organic electronics based on the self-assembly of charge-transfer complexes.

References

[1] K. Müller et al., submitted.

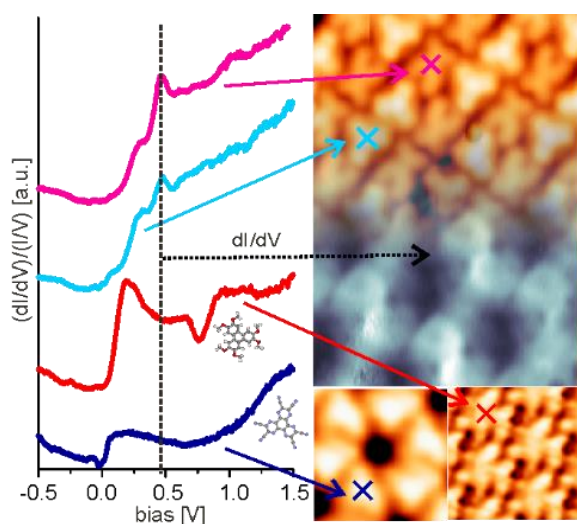


Figure 1: STS data for the homomolecular HATCN and HAT islands (dark blue and red curve, respectively) and for the HATCN (light blue) as well as HAT (pink) molecule in the intermixed layer acquired at 5 K. The panel on the right shows the corresponding STM images and simultaneously acquired dI/dV map.