Core levels and frontier orbitals of K-doped sumanene monolayer

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Introduction

Although alkali metal adsorption of the aromatic molecules is a basic model system of the doped organic semiconductors, many things concerning these systems have still been left unsolved. One of the major problem would be the lack of the structural information of the doped system. Therefore, a combination of the structural determination using direct observation and photoemission will be highly necessary to understand the electronic structure of the doped systems.

Experiment

We focused on the monolayer of the bowl-shaped sumanene molecule (Fig. 1). Based on the determination of the molecular structure of the K-doped sumanene monolayer by STM at room temperature, we discussed the origin of the characteristic of the core levels and frontier orbitals in the synchrotron photoemission spectra. UPS was conducted at the BL-2B of UVSOR and XPS was done at BL-13B of Photon Factory.

Results

Fig. 2 shows the STM image of K-doped sumanene monolayer on Ag(111). Sumanene monolayer on Ag(111) consists of bowl-up (convex) and bowl-down (concave) molecules. It is found that K atoms were effectively adsorbed in concave side of sumanene. This observation ensures the sumanene molecule is doped one by one, and K interact directly to the π orbital of sumanene. Upon this discrete doping, C 1s spectra (Fig. 3) showed splitting, while HOMO peak showed continuous shift toward higher binding energy (Fig.4), with increasing doping level. Finally, new state just below the Fermi level was observed which in possibly due to filled LUMO. It is also important to note that the same trend has been observed in the doping of coronene and picene monolayers, where phase separation of the doped area has also been seen[1]. The strictly different behavior of the core level and frontier orbitals upon the K doping could reflect the localized and the delocalized natures of the wave functions, respectively.

$C_{21}H$

Fig. 1 Sumanene

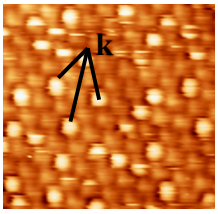

Fig. 2 STM image of K-doped sumanene/Au(111)

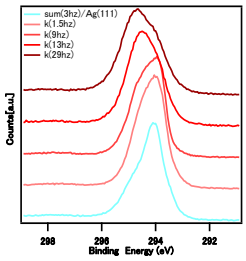

Fig. 3 C 1s spectra of K-doped sumanene/Ag(111)

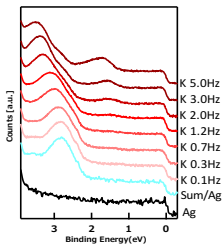

Fig. 4 HOMO spectra of K-doped sumanene/Ag(111)

[1] M. Yano, et al., J. Chem. Phys. 141, 034708 (2014)