Geometric and Electronic Structures of Azobenzene, Azobenzene-derivatives, Pentacene and Rubrene

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Functional molecules have drawn much attention for their possible application to electronic and optical devices. In a chain form, they reveal asymmetric current-voltage characteristics and sometimes switching behavior. So far, the geometric structures were studied with Raman spectroscopy and 2-D time resolved spectroscopy. Scanning tunneling microscopy and spectroscopy has become the most important to tool to understand the structure and electronic structures. Not only their own structures but also their interface with metallic contacts can be studied with this technique. We decide to study semiconducting molecular chains and molecules which reveal conformal transformation with an excitation of light or electrons. Isolated or ordered molecules of azobenzene, azobenzene-derivatives, pentacene and rubrene were studied with scanning tunneling microscopy and spectroscopy. Spatially resolved electronic structures give much information on the substrate-molecule interaction and the inter-molecular interactions. The geometric structures, the registries on metal surfaces and dynamics during a conformal transformation were also studied. Depending on the registries on metal surfaces and the transformation pathways in space and time were found to be different for isolated molecules and ordered molecules due to their molecule-molecule interactions. HOMO, LUMO and HOMO or LUMO derive states on metal surfaces were mapped spatially to find the correlation between bonding with neighboring molecules and the conformal transformation. For isolated molecules, the distance dependence of an inter-molecular interaction can be directly measured by attaching alkyl chains between two molecules. These STM/STS results show good agreement with the DFT calculation results.

[1] B.-Y. Choi, S.-J. Kahng, S. Kim, H. Kim, H. W. Kim, Y. J. Song, J. Ihm and Young Kuk, "Conformational Molecular Switch of Azobenzene Molecule: A Scanning Tunneling Microscopy Study," Phys. Rev. Lett. **96**, 156106 (2006).