Energy-level Alignment of Chemisorbed Monolayers on Metal Surfaces: Implications for Molecular Electronic Junctions

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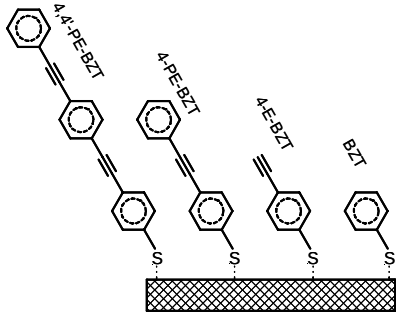
Charge-transport through the interface is a key part of the behavior of any electronic junction. One specific interface property important to molecular-electronic junctions is the energetic alignment of the frontier molecular orbitals relative to the Fermi level of the contact material.

This poster will discuss the energy-level alignment of "molecular wires" chemisorbed on metal surfaces. One-photon, two-photon, and inverse photoemission spectra have been used to determine the energy-level alignment for well-characterized self-assembled monolayers of *para*(phenylene-ethynylene) oligomers chemisorbed on metal surfaces.[1-2]

The valence electronic structure of the chemisorbed monolayer is established by comparing the monolayer spectra to those of the isolated molecule.[3] The effects of molecular length, linker group (thiol and isocyanide), and substrate (copper, silver, gold, platinum) on the energy-level alignment will be presented.[4-6] The observed alignment and its trends can be qualitatively understood in terms of the material properties and a localized interface dipole.

The implications of these results for the design of molecular-electronic devices will be considered.



Self-assembled monolayers studied in this investigation: 4,4'-bis-(phenylethynyl)benzenethiol (4,4'-PE-BZT), 4-(phenylethynyl) benzenethiol (4-PE-BZT), 4-ethynylbenzenethiol (4-E-BZT), and benzenethiol (BZT).

References:

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