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Control of band alignment through coupling chemistry in prototypical molecular wire systems S.W. ROBEY, C.D. ZANGMEISTER, R.D. VAN ZEE, NIST-Gaithersburg, MD — The performance of conjugated molecular systems in electronic applications, either for organic light emitting diodes (OLED's) and field effect transistors, or in more speculative applications proposed for molecular electronics, depends critically on coupling at the molecule-electrode interface. Interactions at this interface determine the alignment of the contact Fermi level with the transport levels in the molecular system and control charge injection into the molecular π levels. We have used one-and two-photon photoemission to examine the influence of coupling chemistry on Fermi level alignment and electronic structure in the prototypical molecular wire, 4,4'-(ethynylphenyl)-1- benzenethiol on Au. These studies reveal a rigid shift of the Fermi level relative to the valence and C (1s) levels upon substitution of the isocyanide coupling for thiol without significant modifications to the overall spectral shape. Absorption measurements reveal no change in optical band gap. These results indicate that substitution of the isocyanide linking chemistry for thiol shifts E_f away from the highest occupied level in the molecule by about 0.5 eV, with little modification of the extended π electronic structure. The interaction at the Au-thiol-OPE interface will be compared and contrasted with the Au-isocyanide-OPE interface in terms of bonding and charge transfer effects and contact made to RAIRS and transport data for related systems.

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