Supplementary Information

Direct aryl-aryl coupling of pentacene on Au (110)

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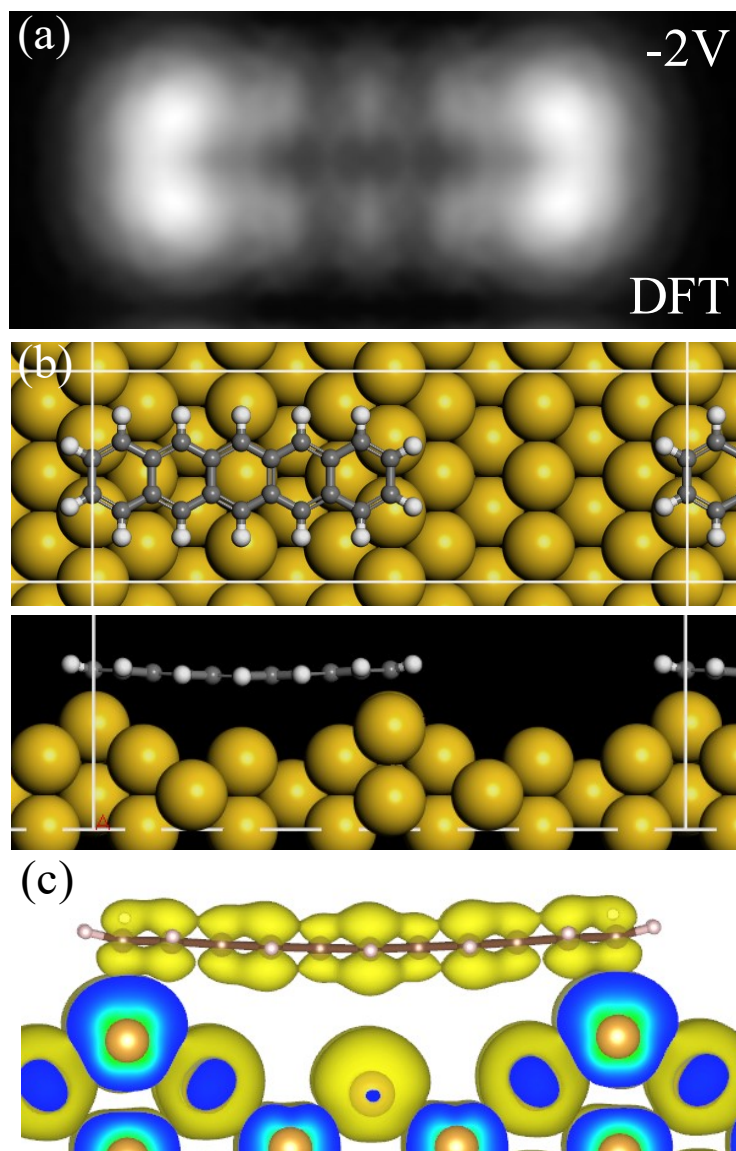
Fig. S1. (a) The DFT-simulated STM image of geometrically optimized pentacene molecule on (1×3) grooves of Au(110). The simulated STM images were obtained by integrating the charge density between the Fermi level and the set bias voltage. (b) The corresponding top views and side views. (c) The corresponding charge density distributions in real space.
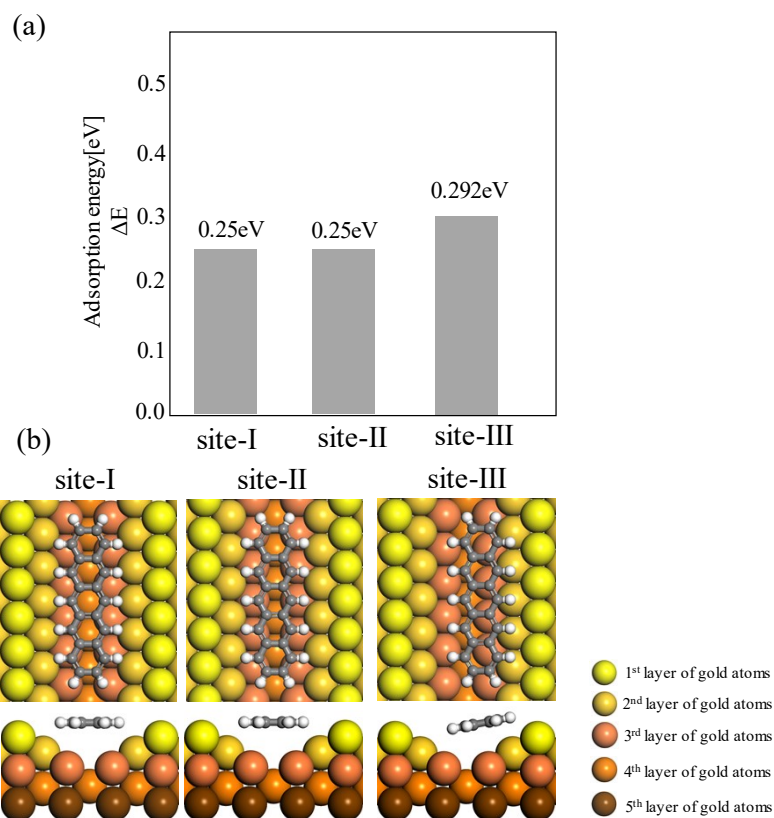
Fig. S2. (a) The adsorption energies of three different adsorption sites of the Au(110) surface without an extra row of gold atoms in the (1x3) groove. (b) Front view and side view of three different adsorption sites. The adsorption energies of site-I, site-II, and site-III are very close.
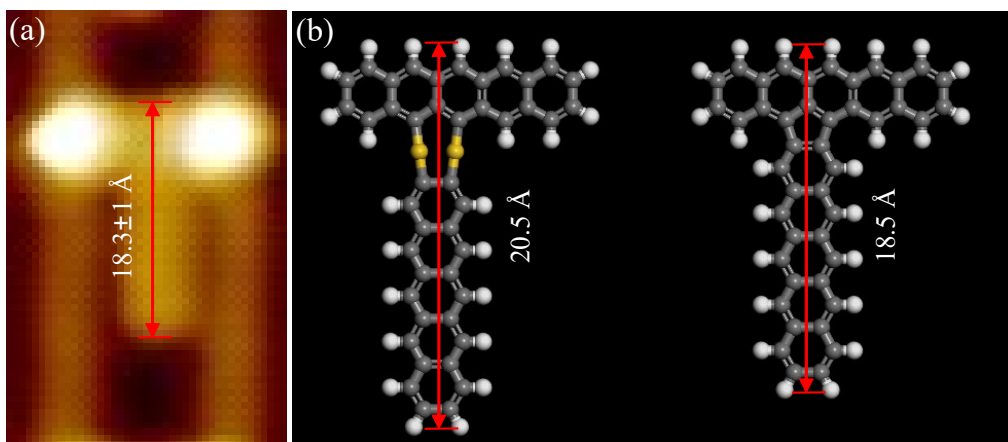
Fig. S3. (a) The actual measured length of the T-shaped dimer. (b) The theoretical lengths of the T-shaped dimers with C-Au-C bonding and with C-C bonding, respectively.
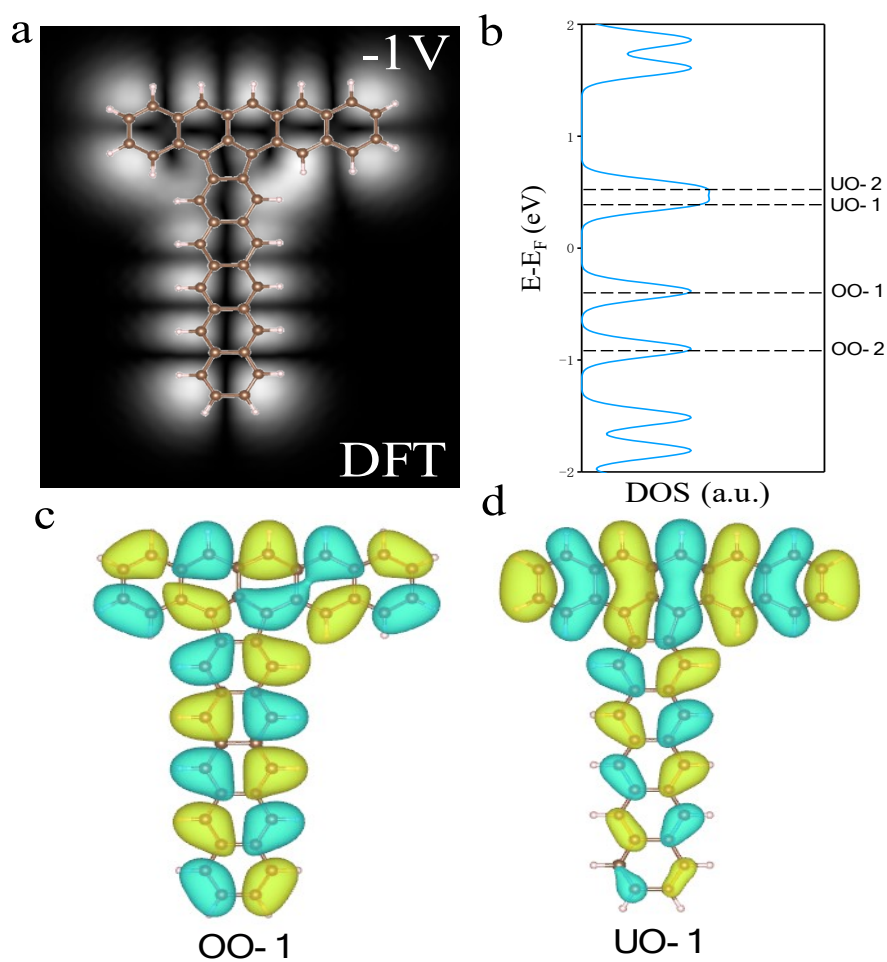
Fig. S4. (a) Optimized molecular model and STM-simulated image of the T-shaped dimer. (b) The calculated DOS of the T-shaped dimer. The dotted lines represent the frontier orbitals of the T-shaped dimer. (c) The wave function of OO-1 in real space. (d) The wave function of UO-1 in real space.