Supporting Information of

Lattice-Directed Construction of Metal-Organic Molecular Wires of Pentacene on Au(110) Surface

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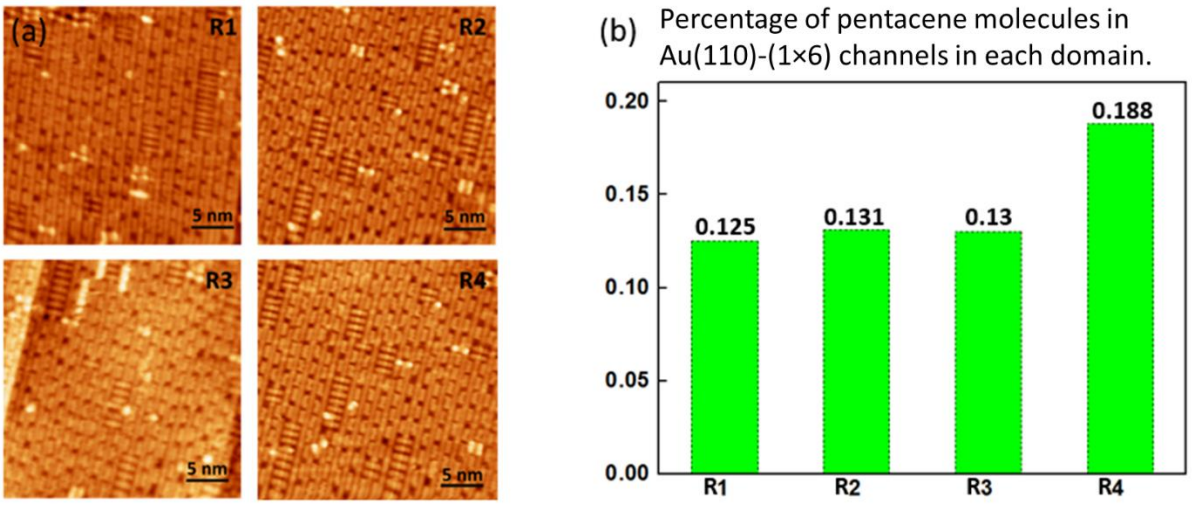

Figure S1, the STM images of several domains and the percentage of pentacene molecules in Au(110)-(1×6) channels in each domain.

We conducted the statistical analysis on the overall percentage of both Au(110)-(1×3) and Au(110)-(1×6) surface reconstruction. We found that the Au(110)-(1×3) surface reconstruction with molecular adsorption predominates with about 80%. We have also found that the (1×3) and (1×6) phase can coexist on Au(110), as shown in Figure S1.

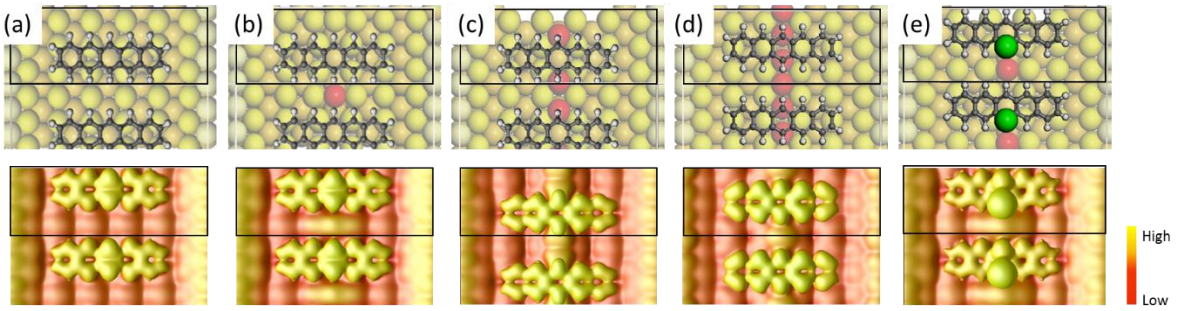

Figure S2, the structures considered for Au(110)-(1×6) reconstruction. (a) pure pentacene molecules, (b) one Au atom between molecules, (c) two Au atoms, (d) three Au atoms and (e) Au adatoms above the molecule.

We determine the structural model based on whether the simulated STM image matches the experimental ones. We considered several configurations, such as pure pentacene molecules (Figure S2a), one Au atom between molecules (Figure S2b), two Au atoms (Figure S2c), three Au atoms (Figure S2d) and Au adatoms above the molecule (Figure S2e). The corresponding simulated STM images are shown in the lower panels in Figure S2. We can see the simulation results in Figure S2a are in agreement with the experimental results shown in Figure 2f. The simulation results in Figure S2c are better for 1-D molecular wire of Au adatoms as shown in Figure 3c.