

## Supporting Information

### Electronic Structures of One-dimensional Metal-Molecule Hybrid Chains Studied using Scanning Tunneling Microscopy and Density Functional Theory

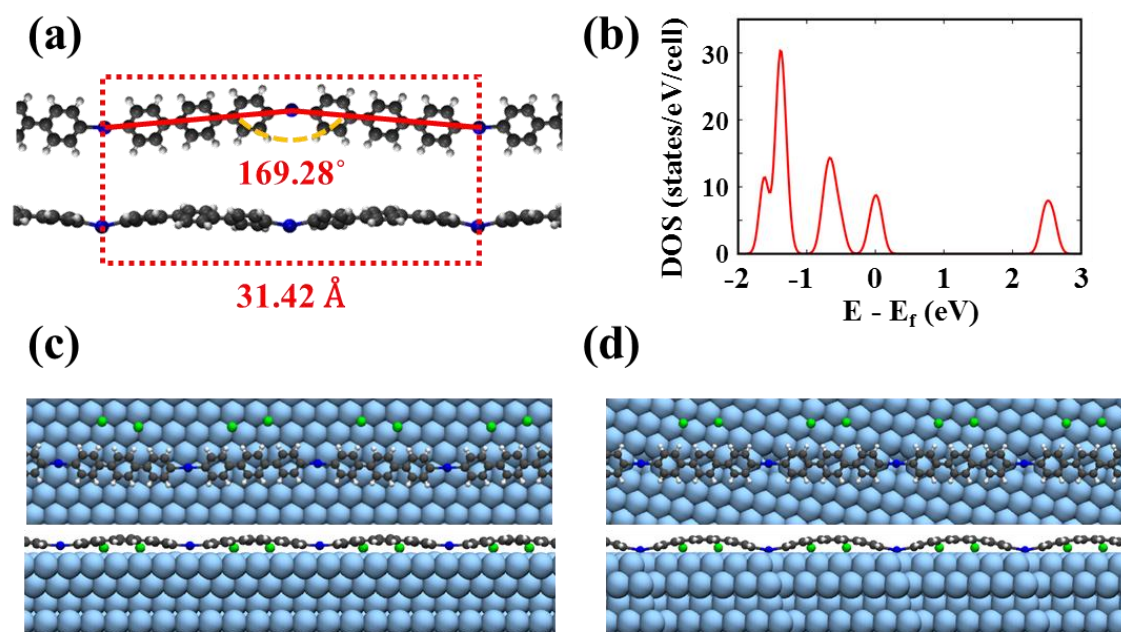
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Equilibrium structures and density of states (DOS) of infinite hybrid chains



**Figure S1.** (a) Equilibrium structure of an isolated (without Ag substrate) infinite Ag-TP chain with two formula units in the unit cell. Despite there is no Ag surface, the chain is not straight and flat, but tilted and concaved down. (b) Density of states (DOS) of the equilibrium structure shown in (a). The degenerate states are half-filled at the Fermi level showing the metallic character. There is an energy gap of about 2.5 eV from the Fermi level to the lowest unoccupied state. The size of this energy gap appears to be kept when this hybrid chain is placed on the Ag(111) surface. Two relaxed atomic configurations with (c) adatom-like Ag and (d) embedded Ag to surface. The structure of (c) is more stable than individual DBTP molecules on the Ag substrate by  $\sim 1.6$  eV. That of (d) is less stable than individual DBTP molecules on the Ag substrate by  $\sim 1.7$  eV. All energy values are given per formula unit of the hybrid chain.