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Supplementary Information

Diacetylene Linked Anthracene Oligomers Synthesized by One-Shot Homocoupling of Trimethylsilyl on Cu(111)

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Figure S1. More coverage of 9,10-bis((trimethylsilyl)ethynyl)anthracene (TMSEA) on Cu(111). (a) Scanning tunneling microscopy (STM) topography. Deposited TMSEA forms one-dimensional structure mostly. (b) Atomic force microscopy (AFM) image. Blue and red arrows indicate anthracene backbone and the trimethylsilyl (TMS) group. The molecules are most probably condensed by the van der Waals interaction between the TMS groups. Measurement parameters: Bias voltage $V_{\text{tip}} = -200$ mV, tunneling current $I = 1.5$ pA in A and $V_{\text{tip}} = 0$ mV and oscillation amplitude $A = 50$ pm.

Figure S2. Simulation results for possible configurations of the isolated TMSEA on the Cu(111) surface with relative adsorption energies of (a, b) +1.62 eV, (c, d) +1.38 eV and (e, f) +0.45 eV to the lowest energy configuration (g, h).
Figure S3. (a) Lowest energy configuration of TMSEA adsorbed on Cu(111) with one of the top-most methyl groups without any rotation, calculated with density functional theory (DFT) calculations. (b-e) A series of simulated AFM images at different heights based on this relaxed molecular structure. This images are taken at the same tip-heights as in Fig.1(h-k) in the main text.
Figure S4. Simulation results for the isolated TMSEA on the Cu(111) surface. Lowest energy relaxed structure from the (a) top and (b) side, (c) plot of charge of adsorbed system, where red is negative and blue is positive (plotted range -0.8e:2.8e), (d, e) differential charge density upon adsorption at contours of -0.006 eÅ⁻¹ (blue) and 0.001 eÅ⁻¹ (red) and (f) simulated constant current STM at -0.2 V.

Figure S5. (a) STM topography AFM image of single TMSEA and (b) the same image with a narrow contrast. Measurement parameters: $V_{\text{tip}} = -200$ mV, tunneling current $I = 5$ pA.
Figure S6. Formation of five-membered ring. (a) AFM image of the conjugate with anthracene units and (b) possible chemical structure. (c) Another example of the conjugation and (d) corresponding chemical structure. Measurement parameters: $V_{\text{tip}} = 0 \text{ mV}$ and oscillation amplitude $A = 50 \text{ pm}$. 
Figure S7. Plot of the charge of the oligomer system, where red is negative and blue is positive (plotted range -0.2 e:0.2 e), for (a) the polymer on Cu(111), (b) isolated oligomer and (c) isolated oligomer in the relaxed adsorption structure of (A).