Electronic Supplementary Information (ESI)

Linear dislocation tunes chirality: STM study of chiral transition and amplification in a molecular assembly on an HOPG surface

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Experimental Section

DTCD was home-synthesized and dissolved in tetrahydrofuran (HPLC grade, Aldrich) at a concentration of less than 10^{-4} M. The self-assembled monolayers were prepared by depositing a drop of above solution onto a freshly cleaved surface of HOPG (quality ZYB, Digital Instruments) and dried in air.

STM experiments were performed on a NanoScope III SPM (Digital Instruments, Santa Barbara, USA) at ambient conditions. The tunneling tips were prepared by mechanically cutting Pt/Ir wire (90/10). All the images were recorded in the constant-current mode and shown without further processing such as Fourier transformation. The specific tunneling conditions are given in the figure captions.

For theoretical simulation, Materials Studio 3.1 (Accelrys, San Diego, USA) and HyperChem 6.0 (Hypercube Inc., Florida, USA) were employed. Packing models of the two molecules were built by using HyperChem 6.0.

In Fig. S1a, a molecular dislocation can be clearly seen indicated by a blue dashed line. The dislocation is formed by molecular dimers (illustrated by filled pink ovals) alternately added between tetramers along the dashed line. The appearance of dimers changes the continuity of the molecular row with a molecular position displacement along line 1-1' in Fig. S1a. However, no change of chirality can be seen. Two neighbouring domains have the same chirality. Fig. S1b is a structural model showing the molecular arrangement in domain boundary. Molecular dimers (indicated by filled red ovals) can not interrupt the propagation of **S**-type chirality. The chirality is amplified across the fault and over the surface.

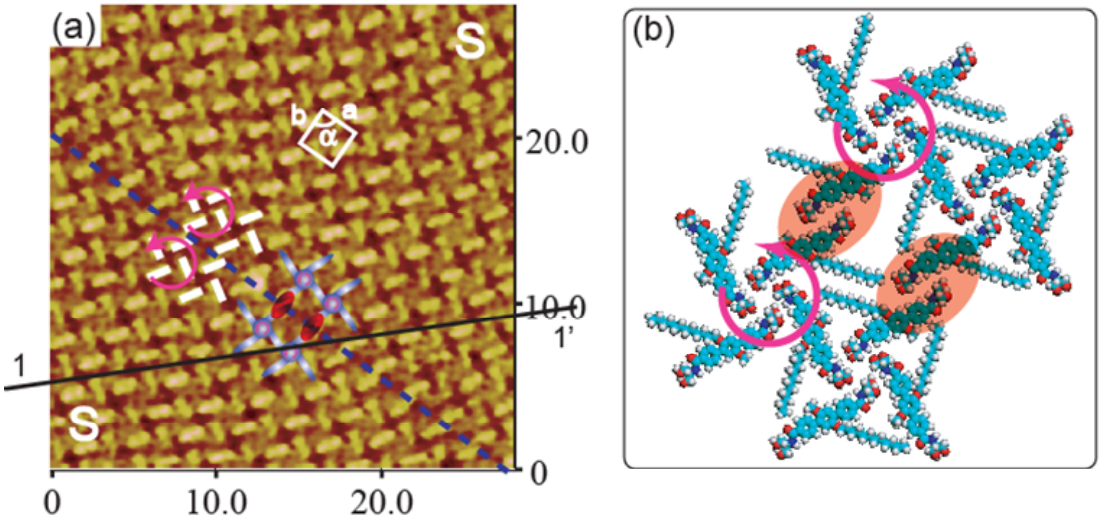

Fig.S1 STM image showing **S-S** domain boundary across a fault dislocation (a) and the structural model (b). Tunneling conditions: E_{bias} = 837 mV, I = 582 pA.