Supporting Information

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Chiral Pinwheel Clusters Lacking Local Point Chirality

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Procedure of DFT calculation:
Density function theory (DFT) in the generalized gradient approximation (GGA) was used to calculate the electronic density of a free pentacene molecule. A double-numerical basis set, together with $d$-polarization functions (DNP), was chosen to describe the electronic wave functions. The Becke exchange functional (B88) in conjunction with the Lee-Yang-Parr correlation functional (BLYP), combined with a DFT-basis relativistic semi-core pseudopotential (DSPP) was used during the optimization. Self-consistent field (SCF) calculations were done with a convergence criterion of $10^{-6}$ hartree on the total energy and electron density.

Figure S. 1: STM images of irregular pentacene pinwheels. a) A R-pinwheel containing some defects (indicated by the arrow). b) A L-pinwheel with a dislocation (marked by the arrow). c) and d) show two irregular pinwheels with six different lobes. All the scale bars correspond to a length of 2 nm.
Figure S. 2: Three sequential images illustrating the robustness of pentacene pinwheels by low bias scanning at $-0.5 \text{ V}$ (18 nm $\times$ 18 nm). From a) to b), the pentacene hexamer B changed to a pentamer B’, which reveals no shifting reversion. One pentacene molecule has been removed by STM tip. Meanwhile, three pentacene molecules have been moved from area-A to area-C. From b) to c), the hexamer B has been recovered from pentamer B’ by STM scanning. The three molecules in C position are removed.