Supplementary Information

Template-assisted 2D self-assembled chiral Kagomé network for selective adsorption of coronene

Yi Wang[a,] ‡, Xiaoping Tan,[b,]‡ Peng Pang[a], Bang Li[a], Xinrui Miao[a,]* Xiaohong Cheng[b,]* and Wenli Deng[a,]*

[a]College of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, People's Republic of China.

[b]Key Laboratory of Medicinal Chemistry for Natural Resources, Chemistry School of Chemical Science and Technology, Yunnan University, Kunming 650091, People's Republic of China.

‡The authors contributed to this work equally.

*To whom correspondence should be addressed. E-mail: msxrmiao@scut.edu.cn; xhcheng@ynu.edu.cn, and wldeng@scut.edu.cn

1. S1. Experimental section

S1.1 Sample preparation

2TDT-10 (6-(5'-(4-((3,4,5-tris (decyloxy)benzyl)oxy)phenyl)-[2,2'-bithiophen]-5-yl)-1,3,5-triazine-2,4-diamine) was home synthesized and reported in previous work.[1] COR, 1-octanoic acid, 1-phenyloctane, *n*-tridecane and *n*-tetradecane were purchased from TCI. All these materials were used without further purification. 1-octanoic acid, 1-phenyloctane, *n*-tridecane and *n*-tetradecane functioned as solvent to dissolve 2TDT-10 and COR, and the initial concentrations of 2TDT-10 and COR were controlled around 10^{-4} mol·L^{-1}. The assemblies were prepared by subsequent deposition of the components onto a freshly cleaved HOPG (grade ZYB, Bruker, USA) surface. All experiments were performed at room temperature. 2TDT-10 solution was deposited on HOPG, and then detected by STM. Afterwards, COR dissolved in *n*-tridecane and *n*-tetradecane was added to 2TDT-10 self-assembly Kagomé structure followed by STM detection, respectively. The low concentration of COR solution was controlled below 10^{-6} mol·L^{-1}.

S1.2 STM detection

The STM measurements were performed on a Nanoscope IIIa (Bruker, USA). In this work, all the images were recorded using the constant current mode under ambient conditions. As STM probes, mechanically cut Pt/Ir tips (80/20) were used.

S1.3 DFT calculations

DFT calculations were performed using the Gaussian 09 software package. The full-geometry optimization of the molecule was conducted using the hybrid M06-2X method together with the split-valence polarized 6-31+g(d) basis set.

References:

1. C. Liu, H. Gao, T. Li, Y. Xiao and X. H. Cheng, *J. Mol. Struct.*, 2019, **1193**, 294-302.

Additional STM Data

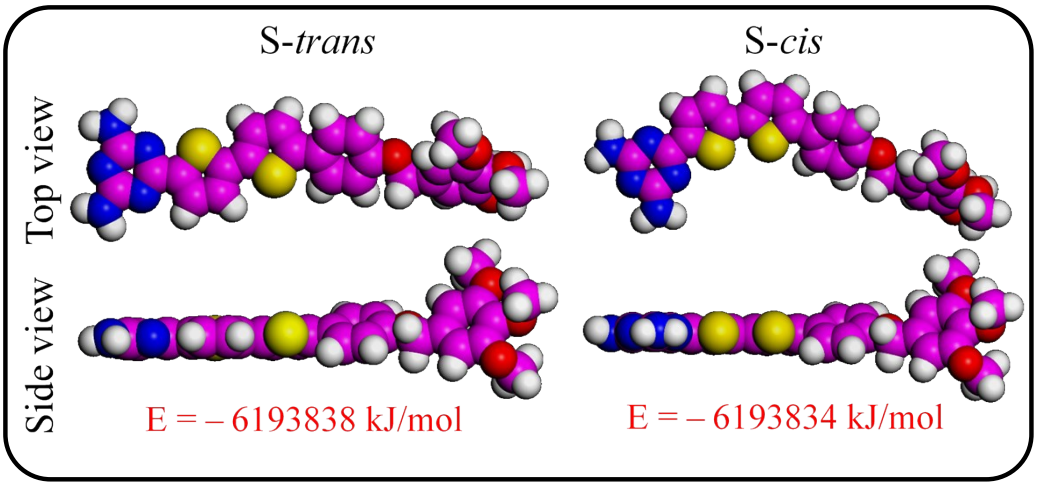

Fig. S1 Scheme of the molecular conformation (the terminal C_{10} chains of 2TDT-10 are replaced by methyl) and corresponding energy. Left: straight *s*-trans conformation; Right: curved *s*-cis conformation. The top and side views of two molecular conformations are presented.

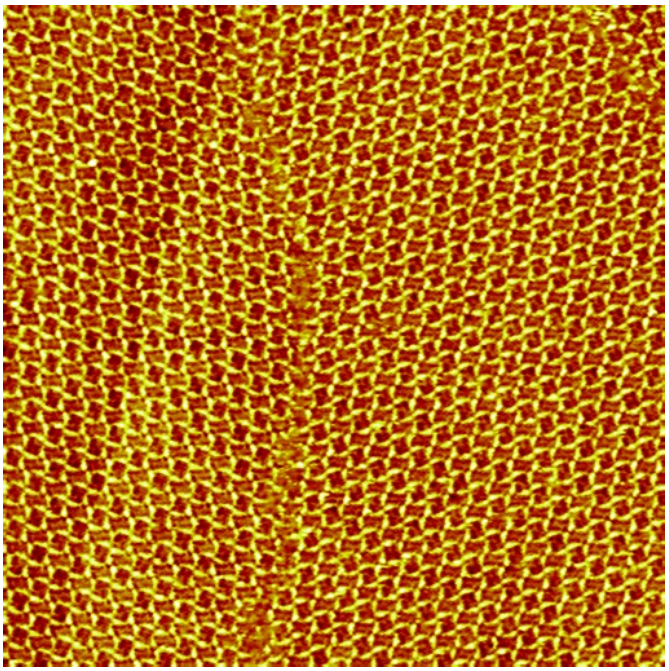

Fig. S2 Large-scale STM image of 2TDT-10 adlayer showing the four-leaved I pattern at the 1-octanoic acid/HOPG interface (90 × 90 nm^2; I_t = 430 pA, and V_b = 500 mV. Concentration: 1.5 × 10^{-4} M).

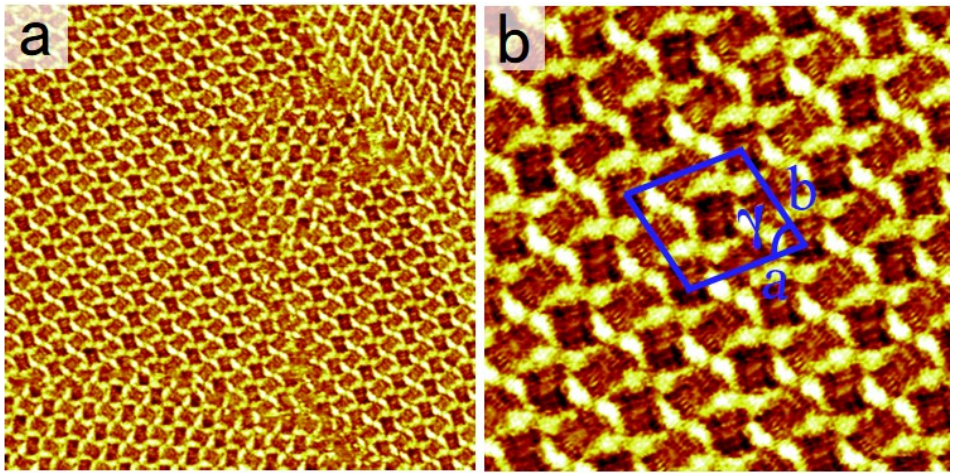

Fig. S3 Large-scale (a) and high-resolution (b) STM images of the 2TDT-10 adlayer showing the four-leaved I pattern at the 1-phenyloctane/HOPG interface (80 × 80 nm^2; I_t = 480 pA, and V_b = 590 mV, 24 × 24 nm^2; I_t = 480 pA, and V_b = 590 mV. Concentration: 1.5 × 10^{-4} M).

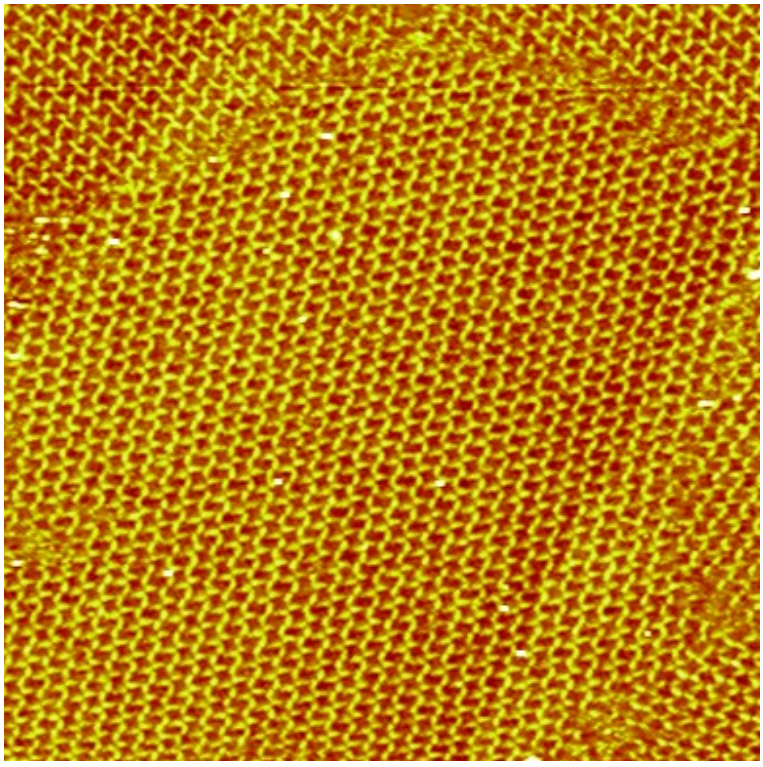

Fig. S4 Large-scale STM image of 2TDT-10 self-assembled nanostructure showing the four-leaved I pattern at the *n*-tridecane/HOPG interface (110 × 110 nm^2; 1.0 × 10^{-4} M; I_t=480 pA, and V_b = 590 mV. Concentration: 1.5 × 10^{-4} M).

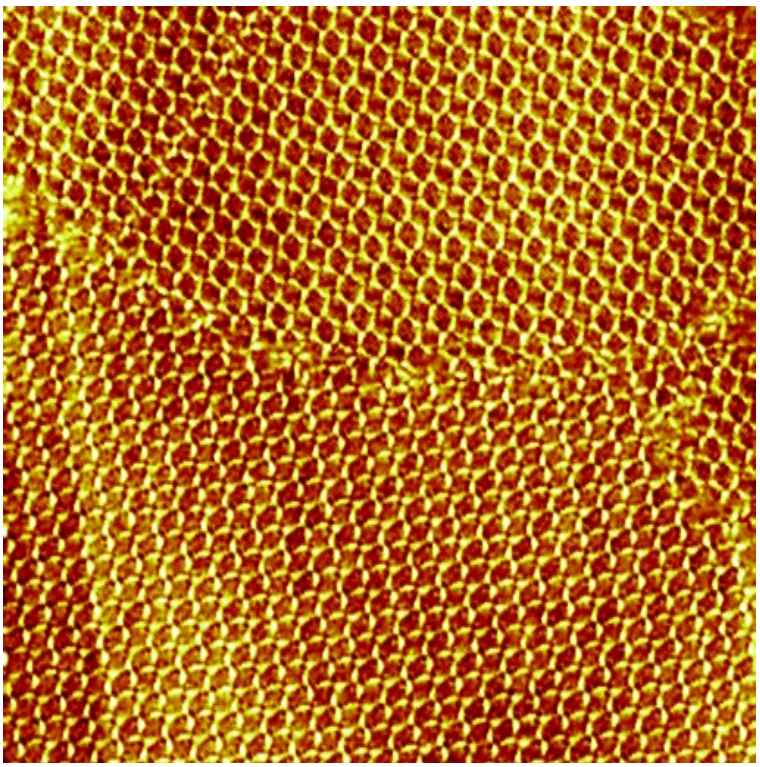

Fig. S5 Large-scale STM image of 2TDT-10 self-assembled nanostructure showing the four-leaved II pattern at the *n*-tridecane/HOPG interface (105 × 105 nm^2; I_t =480 pA, and V_b = 590 mV. Concentration: 2.0 × 10^{-5} M).

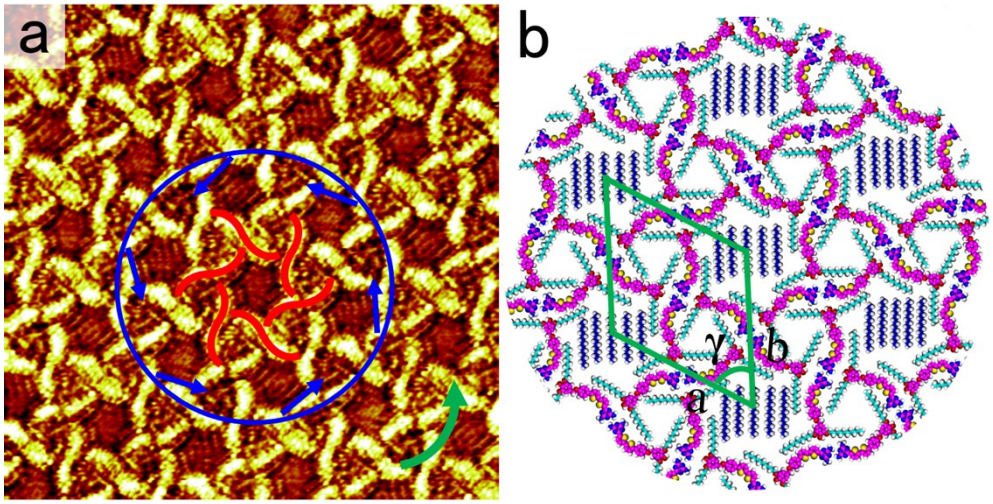

Fig. S6 High-resolution STM image of 2TDT-10 adlayer at the *n*-tridecane/HOPG interface under low solution concentrations. (a) CCW Kagomé pattern: (30 × 30 nm^2; I_t = 480 pA, and V_b = 600 mV; Concentration: 4.0 × 10^{-6} M). (b) Tentative models of CCW Kagomé networks. A unit cell is indicated in green in the model.

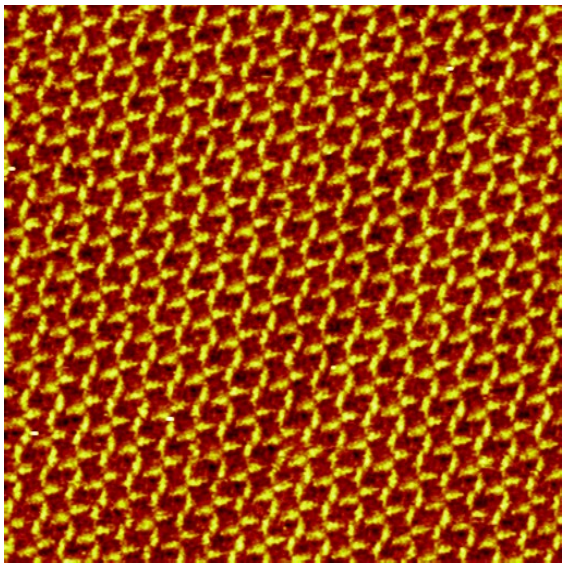

Fig. S7 Large-scale STM image of 2TDT-10 self-assembled nanostructure showing the four-leaved I pattern at the *n*-tetradecane/HOPG interface (67 × 67 nm^2; I_t = 490 pA, and V_b = 580 mV. Concentration: 1.5 × 10^{-4} M).

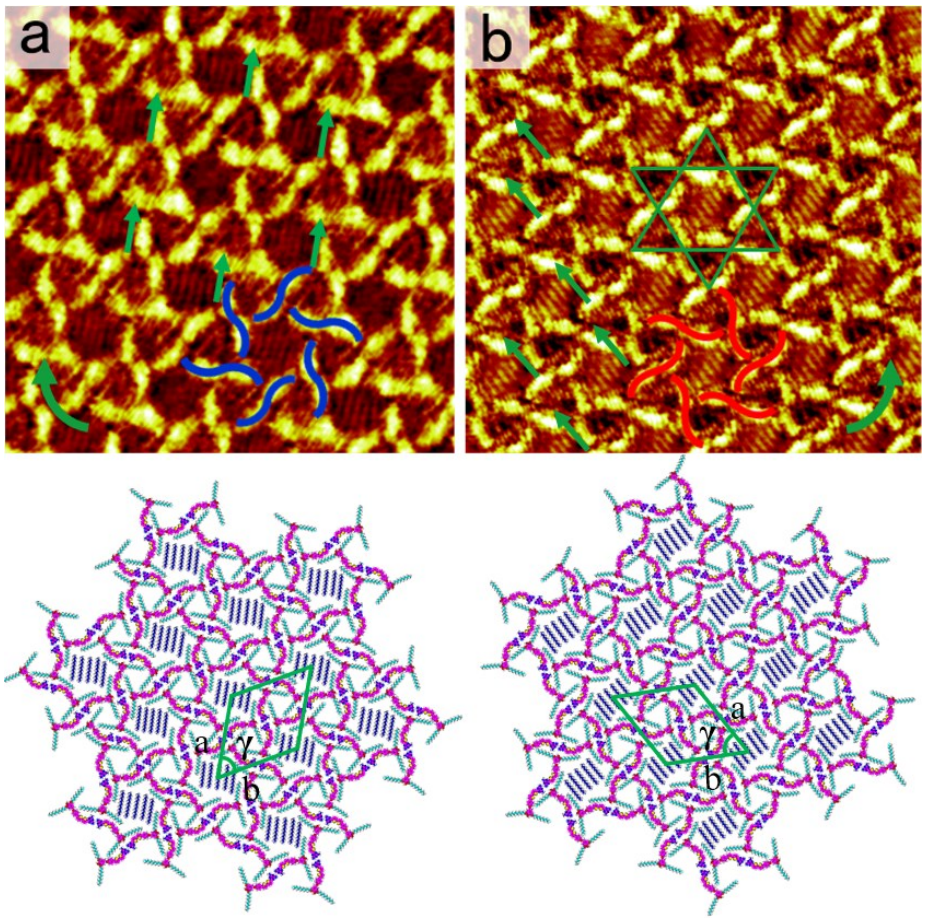

Fig. S8 (a,b) High-solution STM images of 2TDT-10 adlyers at the *n*-tetradecane/HOPG interface with a low solution concentration. (a) CW Kagomé pattern: (24 × 24 nm^2; I_t = 480 pA, and V_b = 600 mV. Concentration: 4.0 × 10^{-6} M). Green straight arrows represent the direction of the co-adsorbed *n*-tetradecane. (b) CCW Kagomé pattern: (24 × 24 nm^2; I_t = 485 pA, and V_b = 610 mV. Concentration: 4.0 × 10^{-6} M). (c,d) Tentative

models of monolayer structure with CW and CCW Kagomé networks, respectively. A unit cell is indicated in green for each model. Green straight arrows represent the direction of the co-adsorbed *n*-tetradecane in (a,b).

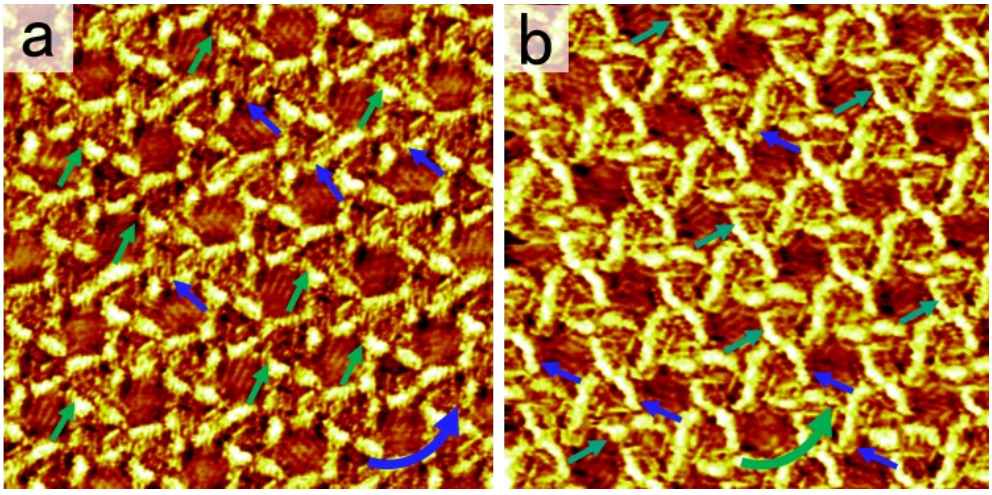

Fig. S9 (a,b) High-resolution STM images of 2T-10 CCW kagomé structures at the *n*-tetradecane/HOPG interface (30 × 30 nm^2; I_t=480 pA, and V_b = 590 mV; Concentration: 4.0 × 10^{-6} M. 30 × 30 nm^2; I_t=460 pA, and V_b = 570 mV; Concentration: 4.0 × 10^{-6} M). Arrow show the different directions of the coadsorbed solvent orientation in the cavities.

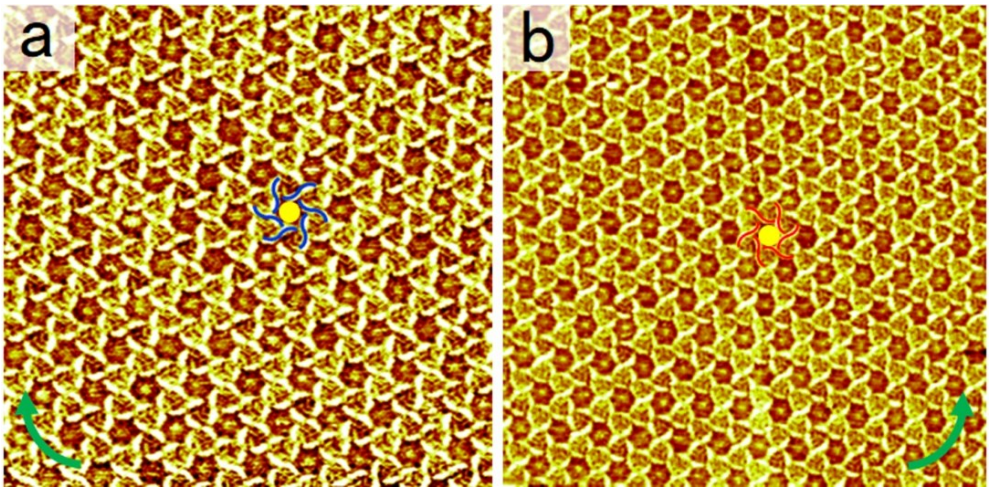

Fig. S10 Large-scale STM images of (a) CW and (b) CCW 2TDT-10/COR (host-guest) Kagomé structures at the *n*-tridecane/HOPG interface. (a) 60 × 60 nm^2; I_t = 480 pA, and V_b = 590 mV; Concentration: 2.0 × 10^{-6} M. (b) 75 × 75 nm^2; I_t = 460 pA, and V_b = 575 mV; Concentration: 2.0 × 10^{-6} M.

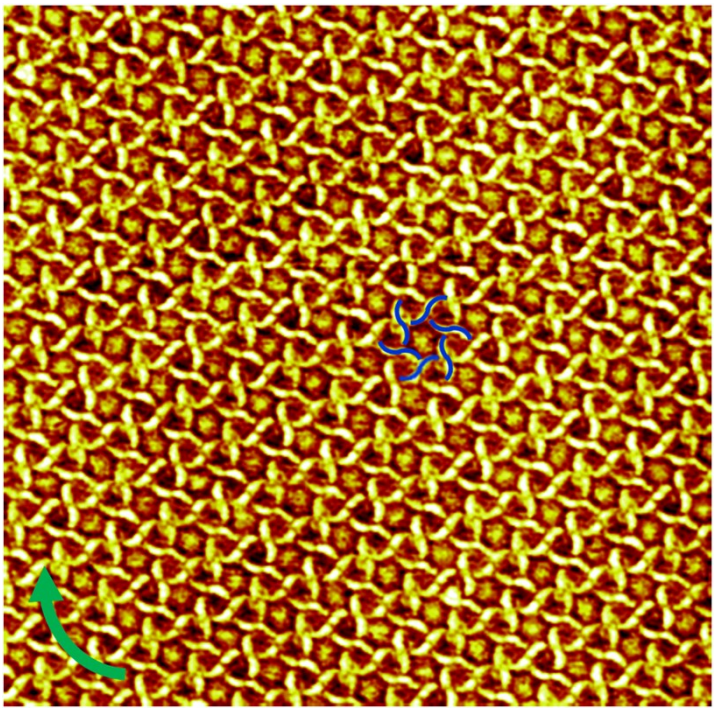

Fig. S11 Large-scale STM image of CW 2TDT-10/COR (host-guest) Kagomé structures at the *n*-tetradecane/HOPG interface. (a) 75 × 75 nm^2; I_t = 480 pA and V_b = 590 mV. Concentration: 2.0 × 10^{-6} M).

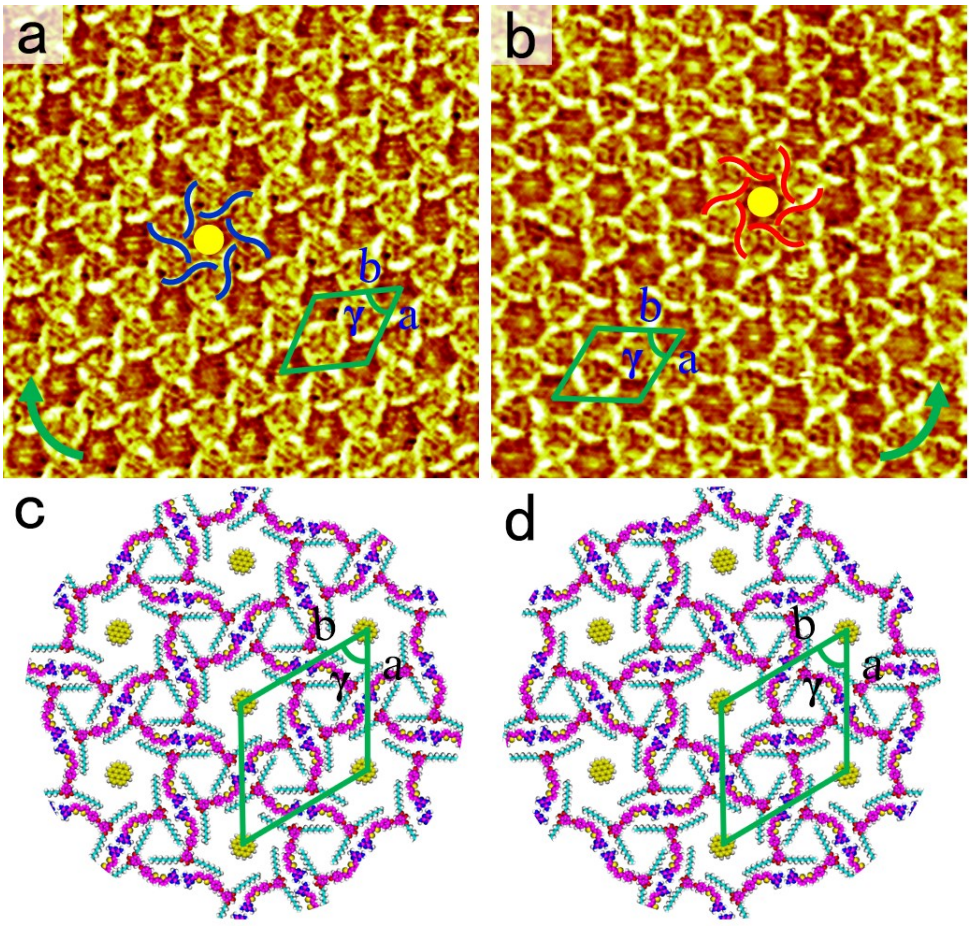

Fig. S12 (a,b) High-resolution STM images showing CW and CCW Kagomé networks of 2TDT-10/COR nanostructures at the *n*-tridecane/HOPG interface. (a) 30 × 30 nm^2; I_t = 450 pA and V_b = 590 mV.

Concentration: 2.0 × 10^{-6} M. (b) 30 × 30 nm^2; I_t = 480 pA and V_b = 570 mV. Concentration: 2.0 × 10^{-6} M. (c,d) Tentative models for host-guest CW and CCW Kagomé networks. A unit cell is indicated in green for each model.

Table S1. Lattice Parameters of Molecular Self-Assembled Patterns for 2TDT-10 under Di□erent Solvents at the Interface.

Structural model	Solvent	*a* (nm)	*b* (nm)	*θ* (°)	N[a]	Area density, S (nm^2 per molecule)
Four-leaved I	Octanoic acid 1-Phenyloctane *n*-Tridecane *n*-Tetradecane	4.5 ± 0.1	6.2 ± 0.1	40 ± 1	4	4.59
Four-leaved II	*n*-Tridecane	3.9 ± 0.1	6.2 ± 0.1	50 ± 1	4	4.73
Kagomé network	*n*-Tridecane *n*-Tetradecane	6.1 ± 0.1	6.1 ± 0.1	60 ± 1	6	5.37
Kagomé (host-guest)	*n*-Tridecane *n*-Tetradecane	6.1 ± 0.1	6.1 ± 0.1	60 ± 1	6 (host) 1 (guest)	-

[a]N stands for the number of molecules per unit cell in each structure.