Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information

A Thermo-driven DNA Zipper

Chunyan Wang, Yu Tao, Youhui Lin, Jinsong Ren*, Xiaogang Qu

Experimental section:

Table S1: All DNA oligonucleotides used in the experiments are listed as follows.

Table S1: sequences used in the experiments

NO.	Sequences
1	*5*'-CACAGCGGTAGCGTGGACTAG-*3*'
2	*5*'-GACTGCCGACTGGTGCTCACCGTAGTTGCTGG-*3*'
3	*5*'-GCAGTACGTGTGGCACAACGGCATGACATACACCGATACGAT-*3*'
4	*5*'-ACTATGCTAGTCCTGTATGTCATGCCGTTGTGCCTGAGCACCAGTCGCG-*3*'
5	*5*'-CTGACGCCAGCAACTACGGACACGTACTGCATCGTATCGGACGCTACC-*3*'
6	*5*'-CGTCAGGCTGCTGTGGTCGTGC-*3*'
7	*5*'-CATAGTCGTCGATACGGCACCATGATGCACG-*3*'
8	*5*'-GCTGTGCGTGCATCATGGACTAACCAGTGGCAAC-*3*'
9	*5*'-CCCCATAACCCCTTTGTTGCTTACCGCATCGGACAGCAGC-*3*'
10	*5*'-GCAGTCGCACGACCTGGCGTTGTACTACGCAATCCTGCCGTATCGACG-3'
11	*5*'-AGTACAACGCCACCGATGCGGTCACTGGTTAGTGGATTGCGT-*3*'
12	*5*'-GGGGTTATGGGGTTTGTTGCTTACCGCATCGGACAGCAGC-*3*'
13	5'-GGACTAGCATAGTTGTGCCGTA-3'
14	5'-CTGACTTACGGCACAGCGGTAGCGT-3'
15	5'-GCTAGTTGGCACAGCGGTAGCGT-3'
16	5'-GGACTAGCATAGTTTTTCCAACTAGCGACTGA-3'
12^{L}	*ROX-5*'-GGGGTTATGGGGTTTGTTGCTTACCGCATCGGACAGCAGC-*3*
8^{L}	*5*'-GCTGTGCGTGCATCATGGACTAACCAGTGGCAAC-*3*'-Dabcyl
17	5'-TGTTGCTTACCGCATCGGACAGCAGC-3'
18	5'-TTTTTTTTTTGTTGCTTACCGCATCGGACAGCAGC-3'

Materials and methods. Tris (tris-hydroxymethylaminomethane) was purchased from USB. All the other reagents used in the experiments were purchased from Sigma. All the DNA oligonucleonides were purchased from Sangon Biotech (ShangHai, China) and purified by HPLC. Concentration of each DNA was estimated by absorption at 260 nm. Molar extinction coefficients were estimated by the nearest neighbor method.

Electrophoresis. The native PAGE experiments were carried out on 8% polyacrylamide (19:1 acrylamide: bisacrylamide ratio) gel and run for 2.5 hours with a field of 80 V at 4 ℃. The running buffer consisted of 50 mM Tris-HCl, pH 8.0, 20 mM acetic acid, and 2 mM EDTA (TAE). Silver staining was applied in the experiments.

AFM (atomic force microscopy). AFM imaging was performed under Tris-Mg buffer in tapping mode under air on a Multimode V using NP-S tips (Veeco Inc.) with a scan rate of 1Hz, 512*512 lines. 10μL of the diluted DNA assemblies sample at each state (assemblies at 20 ℃, the assemblies that were warmed up to 39 ℃ and cooled down to 20 ℃) were applied immediately to a piece of freshly cleaved mica (as a drop and left to adsorb to the surface for 30 s). Deionized water was added to the drop on the mica to wash off salts afterwards. Finally, the substrate was dried with compressed air. Each sample preparation was controlled under 2 minutes to guarantee the uniform deposition of corresponding conformation on mica.

Fluorescence spectra. Fluorescence measurements were carried out on Jasco-FP-6500 spectrofluorometer (Jasco International Co. LTD. Tokyo, Japan) using a quartz cell of 1 cm path length, with an excitation wavelength of 585 nm. And fluorescence emission spectra were monitored from 595 to 650 nm. The slits for the excitation and emission monochromators were both set to 5 nm. The kinetics of fluorescence intensity changing with time was measured at excitation wavelength of 585 nm, monitored at wavelength of 602 nm. The solution temperature was controlled through a connected thermal controller and water bath.

Formation of individual units. Stoichiometric quantity of each strand in the unit was fixed at a concentration of 5 μM, in TAE/Mg buffer (50 mM Tris·HCl, pH 8.0, 20 mM acetic acid, 2 mM EDTA, and 10 mM magnesium acetate). The solution was

cooled slowly from 95 ℃ to 20 ℃ over 48 hrs and incubated in 4 ℃ for at least 10 hrs.

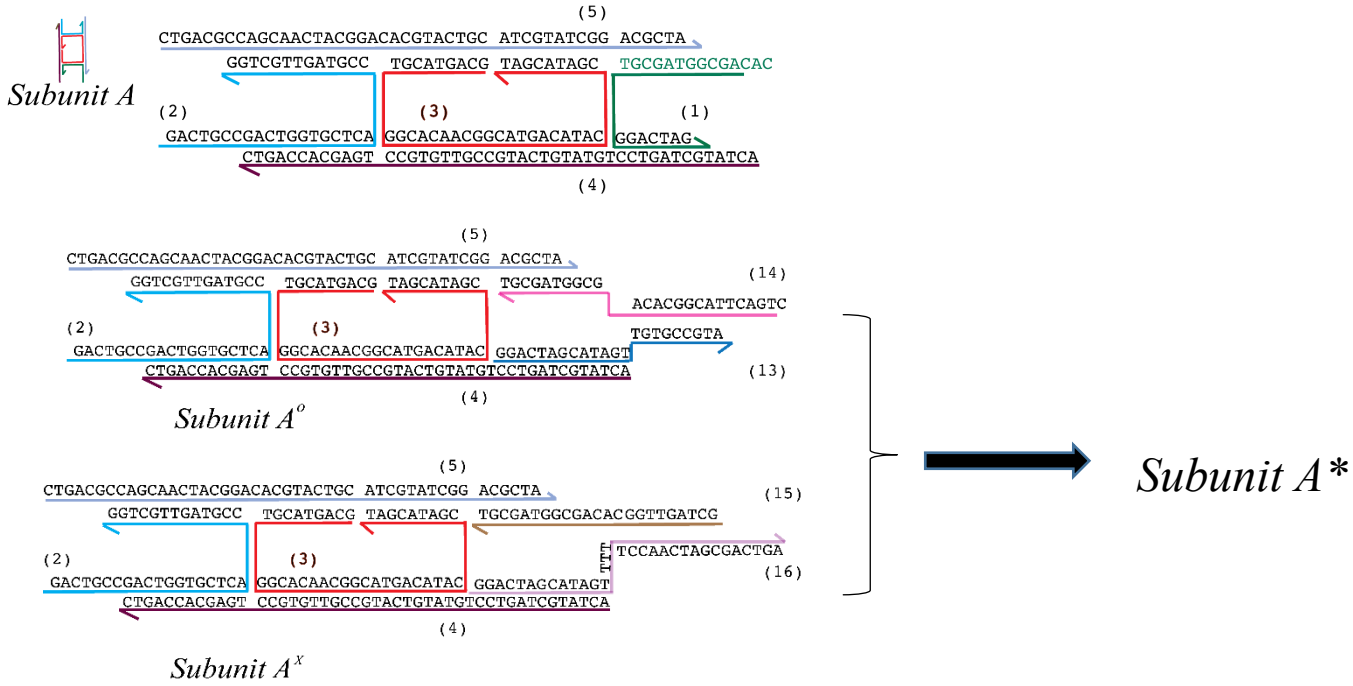

Figure S1. The formation of subunit A, subunit A^o and A^x. The subunits were short for SA, SA^o and SA^x in the main text, respectively. Subunit A is constructed from strands 1-5; subunit A^o is constructed from strands 2-4, strand 13 and strand 14; subunit A^x is composed of strands 2-4, strand 15 and strand 16. Subunit A* is assembled from SA^o and SA^x.

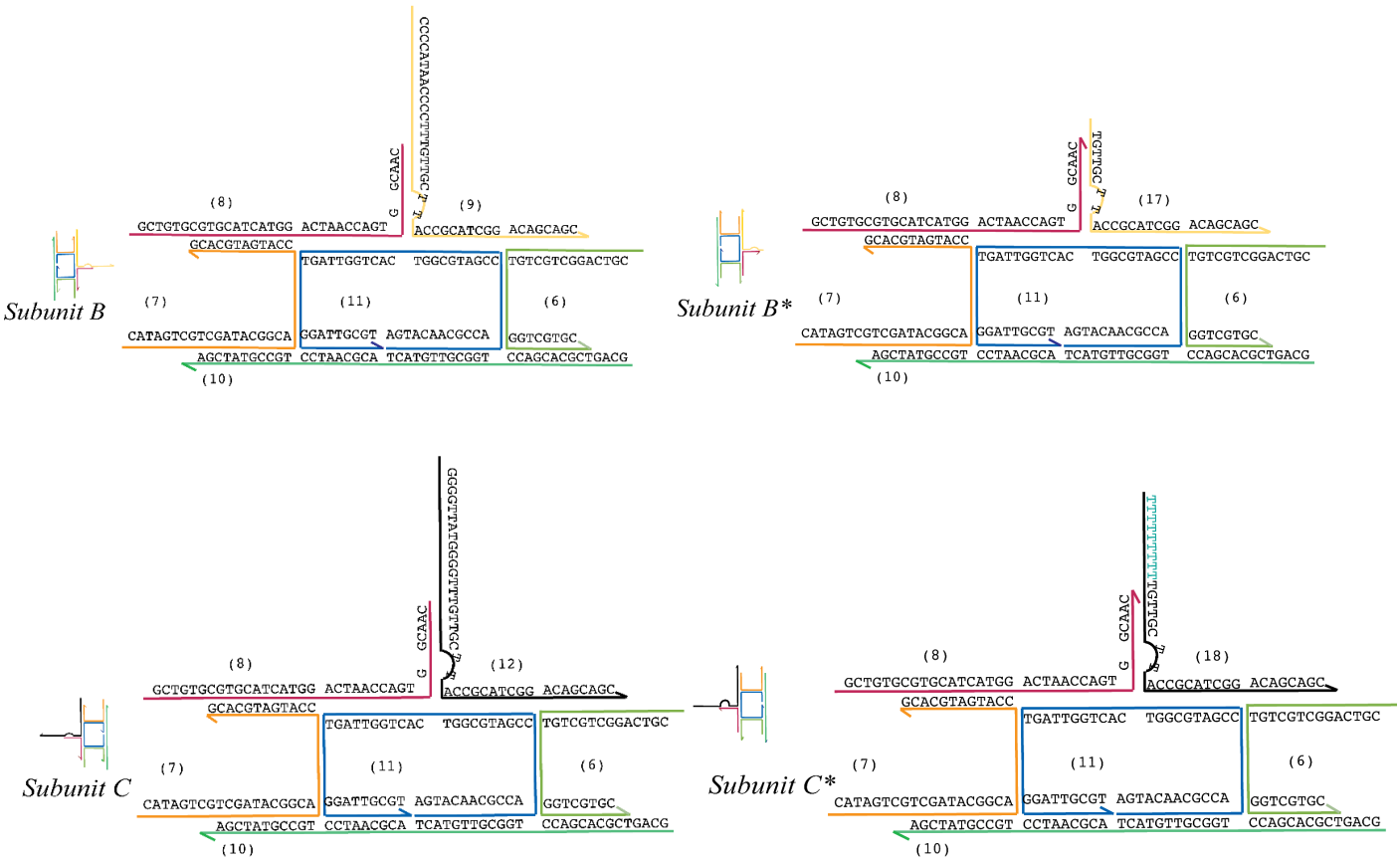

Figure S2. Construction of subunits B, B*, C and C*. Subunit B (SB) is composed of strands 6-11; subunit C (SC) is composed of strands 6-10 and strand 12. Subunit B* contains strands 6, 7, 8 as well as strands 11 and 17; subunit C* contains strands 6, 7, 8, strands 11 and 18.

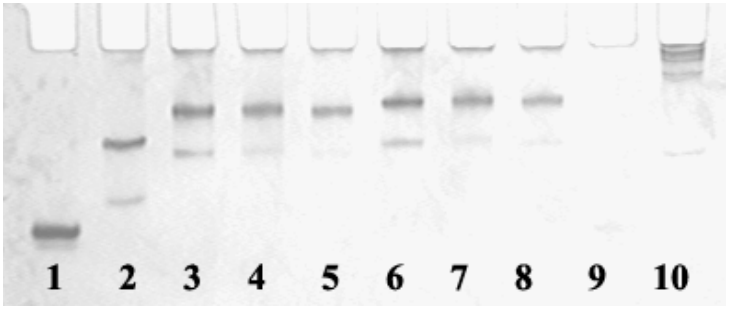

Figure S3: PAGE of the device formed by control units. Lane 1: SA^{o}; lane 2: SC; lane 3: SA^{o}+SB*; lane 4: SA^{x}+SB*; lane 5: (SA^{o}+SB*) + (SA^{x}+SB*); lane 6: SA^{o}+SC; lane 7: SA^{x}+SC; lane 8: (SA^{o}+SC) + (SA^{x}+SC); lane 10: DL 15000.

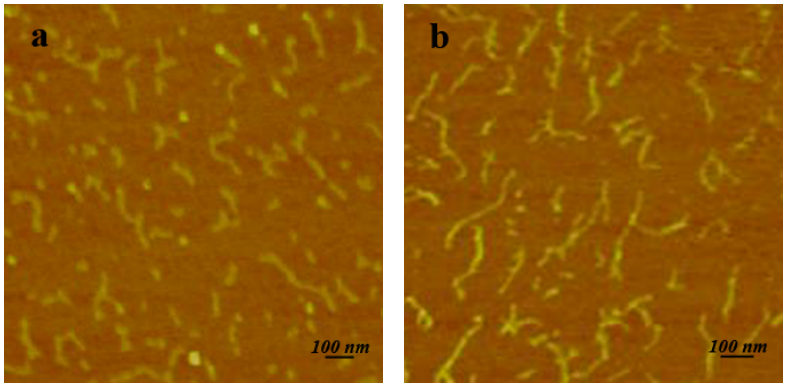

Figure S4: The AFM images of the device formed from control subunits SB* and SC*. A) The device formed by control units at room temperature; b) AFM image of the assembly that formed by control units when the temperature increased to 39 ℃.

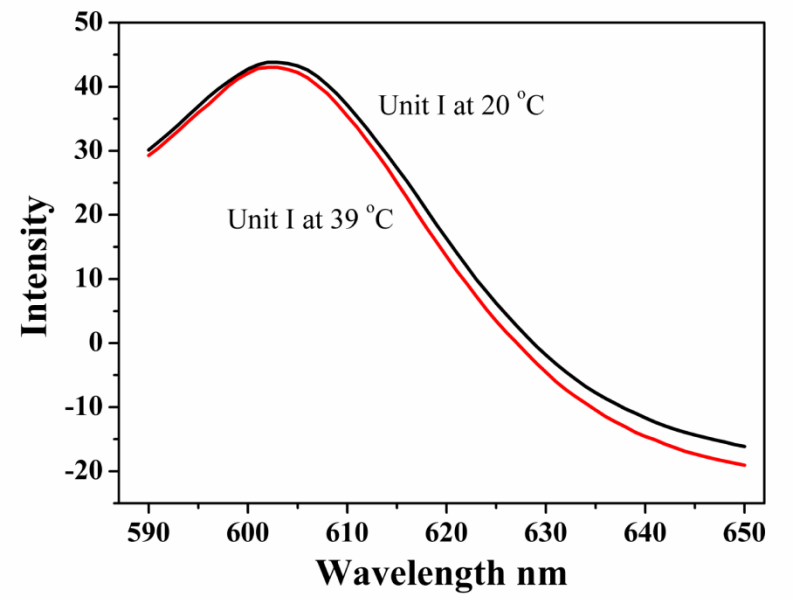

Figure S5: The fluorescence intensity of ROX at 20℃ (black curve) and 39℃ (red curve). The fluorophore ROX is insensitive to the temperature in our experiments.

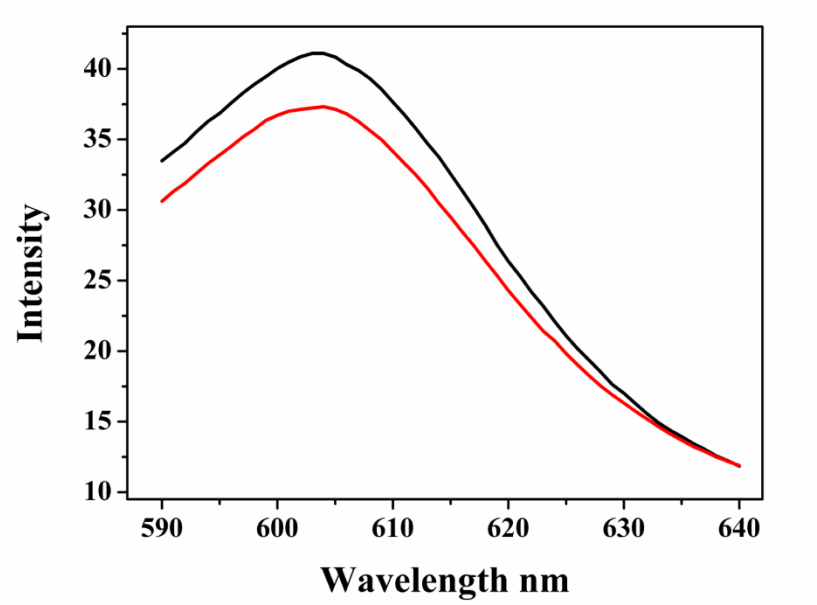

Figure S6: The fluorescence spectra of stripes constructed from control subunits SB* and SC*. Black curve is the fluorescence spectra of one stripe that labeled with ROX; red curve is corresponding to its spectra after mixing with other stripe labeled with Dabcyl.