

Supplementary Information

Force-driven base recognition programs DNA origami-based supramolecular networks

Liqiong Niu,^a Yuanyuan Luo,^a Pengyan Hao,^a Xiaoya Sun,^a Yongxi Zhao^{a,b} and Na Wu *^a

a. Institute of Analytical Chemistry and Instrument for Life Science, The Key Laboratory of Biomedical Information Engineering of Ministry of Education, School of Life Science and Technology, Xi'an Jiaotong University, Xianning West Road, Xi'an, Shaanxi 710049, P.R. China.

b. Frontier Institute of Science and Technology, and Interdisciplinary Research Center of Frontier Science and Technology, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, P.R. China

*Corresponding author. E-mail: wuna2017@xjtu.edu.cn

Experimental Section

Materials

All short ssDNA strands were purchased from Sangon Biotech Co., Ltd. (Shanghai, China). Streptavidin was purchased from Sangon Biotech Co., Ltd. (Shanghai, China). The M13mp18 phage scaffold strand was purchased from New England Biolabs Inc. Tris, acetic acid (CH_3COOH), magnesium acetate ($\text{C}_4\text{H}_6\text{O}_4\text{Mg}$), and ethylenediaminetetraacetic acid (EDTA, $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_8$) were all purchased from Aladdin Biochemical Technology Co., Ltd. (Shanghai, China).

Fabrication of DNA Origami Structures

In this study, hexagonal DNA origami and twist-corrected rectangular DNA origami structures were employed. Hexagonal and twist-corrected rectangular origami structures were designed using caDNAno software (design diagram shown in Fig. S13 and Fig. S14). For preparation, staple strands (including internal and edge staples) were mixed with scaffold DNA at a 10:1 molar ratio in 1×TAE/Mg²⁺ buffer (40 mM Tris, 20 mM acetic acid, 2 mM EDTA, and 12.5 mM magnesium acetate, pH 7.5). The mixture was then heated to 95 °C for 3 min in a thermal cycler, followed by gradual cooling to 25 °C at a rate of 0.1 °C per 10 seconds. The synthesized DNA origami was obtained at a final concentration of 5 nM.

Atomic Force Microscopy (AFM) Imaging

Both rectangular DNA origami samples with 0/1 active edges and hexagonal DNA origami samples with 2 active edges were diluted to a final concentration of 0.25 nM. Streptavidin was then introduced and incubated with the sample for at least 30 minutes to ensure thorough recognition of biotin molecules on the origami structures. 3 μL of DNA origami sample was deposited onto freshly cleaved mica surfaces and allowed to adsorb for 5 min. For hexagonal DNA origami samples with 6 active edges, 30 μL of sample solution was applied to clean mica surfaces and maintained in a constant temperature and humidity environment for 34 hours, with the mica surface kept hydrated throughout the process. AFM imaging was conducted using a Multimode VIII AFM (Bruker Corporation) in liquid tapping mode with NP-S probes (Bruker Corporation) having a spring constant of 0.35 N/m. To identify biotin molecules on the origami, streptavidin was added to the samples and incubated for at least 30 minutes. In thermodynamic experiments, sample solutions were incubated at

preset temperatures for 30 min and brought to target temperatures (25 °C, 35 °C, 45 °C, and 55 °C respectively) using the AFM external heating device prior to measurement to ensure the entire imaging process occurred at predetermined temperatures. Fast Fourier transform (FFT) analysis of AFM images was performed using Nanoscope Analysis 1.9 offline software.

UV Irradiation

The successfully prepared hexagonal or rectangular DNA origami samples were exposed to UVB irradiation (2.0 W/m²) for 10 minutes at 25 °C, with the entire process conducted in an ice bath to prevent sample heating. Following UV treatment, the origami samples were incubated at predetermined temperatures for 30 min prior to AFM imaging.

Yield analysis.

The sample was deposited on mica for AFM imaging. The numbers of monomers and dimers in the AFM images were counted and marked as “M” and “D”, respectively (Fig. S1, S2, S9 and S10). The yield of the dimers was calculated as:

$$Y_{(dimer)} = \frac{2D}{M + 2D} \times 100\%$$

Count the numbers of monomers, dimers and trimers in AFM images marked as M, D and T respectively (Fig. S3, S11 and S12). The yield of the trimers was calculated as:

$$Y_{(trimer)} = \frac{3T}{M + 2D + 3T} \times 100\%$$

For the large-scale assembled structures of DNA origami, we adopted the area ratio calculation method described in Fang's work¹. The total area of the origami structures ($A_{origami}$) and the total imaging area (A_{total}) were calculated separately using imageJ software (Fig. 3 and 4). The relative area of the large-scale assembled structures were calculated as:

$$Y_{(origami)} = \frac{A_{origami}}{A_{total}} \times 100\%$$

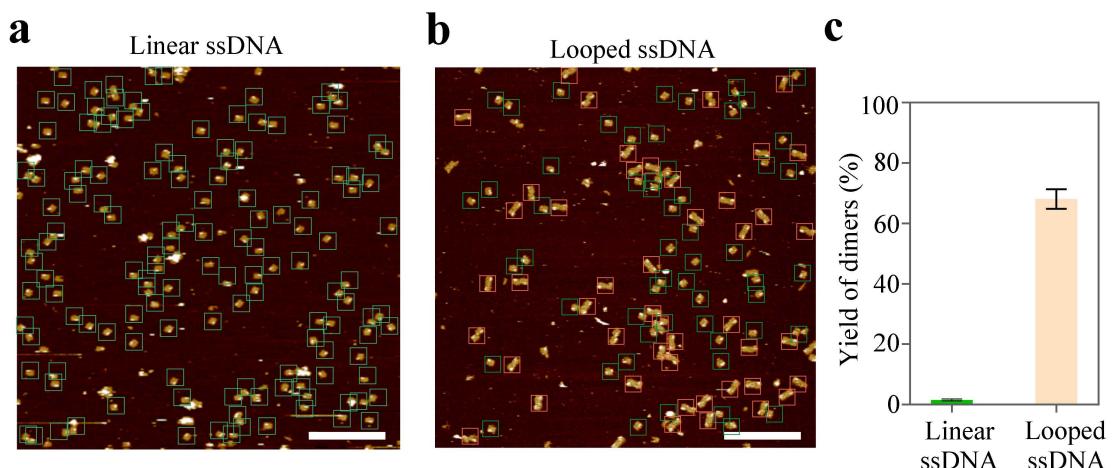
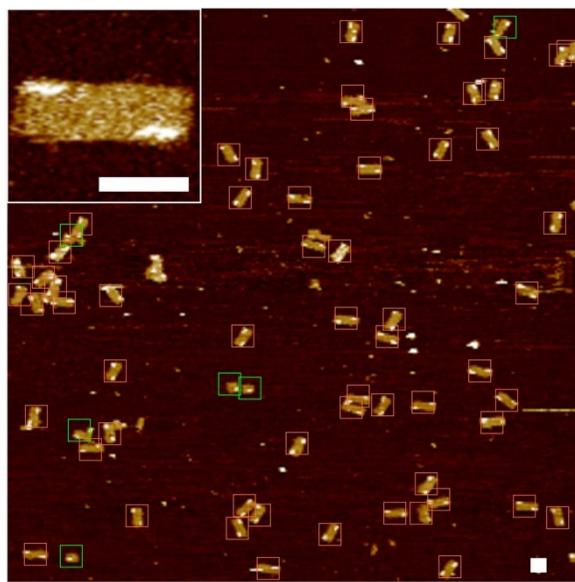
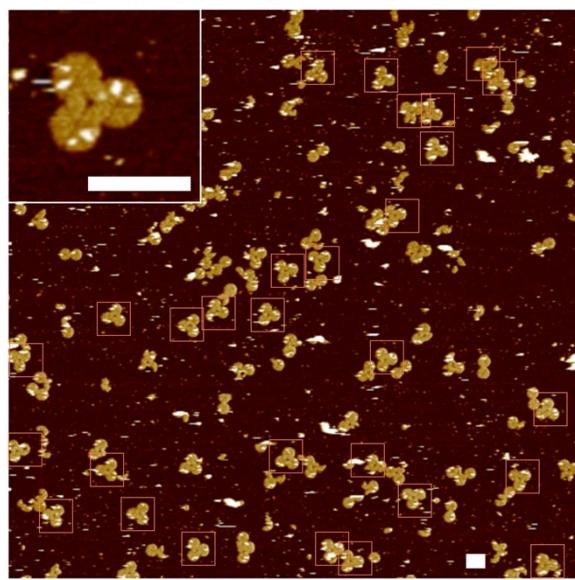


Fig. S1 (a) Representative AFM images of the DNA origami nanostructure with 4-nt polyA linear single-stranded DNA extending from the edge. Scale bars: 1 μm . (b) Representative AFM images of the DNA origami nanostructure with 4-nt polyA loop extending from the edge. Scale bars: 1 μm . (green boxes: monomers; orange boxes: dimers) (c) Histogram showing the yield of dimers mediated by linear ssDNA ($n=202$) and looped ssDNA ($n=187$).



Yield of dimers = $87.2 \pm 2.6\%$

Fig. S2 Representative AFM images of DNA origami dimers mediated by 4-nt polyG loop recognition. The corresponding dimers yields were analyzed from AFM images ($n=197$). Monomers: green boxes. Dimers: orange boxes. Scale bar: 100 nm.



Yield of trimers = $57.3 \pm 3.8\%$

Fig. S3 Representative AFM images of DNA origami trimers mediated by 4-nt polyG loop recognition at two adjacent active edges. The corresponding trimers yields were analyzed from AFM images ($n=179$). Trimers: orange boxes. Scale bar: 200 nm.

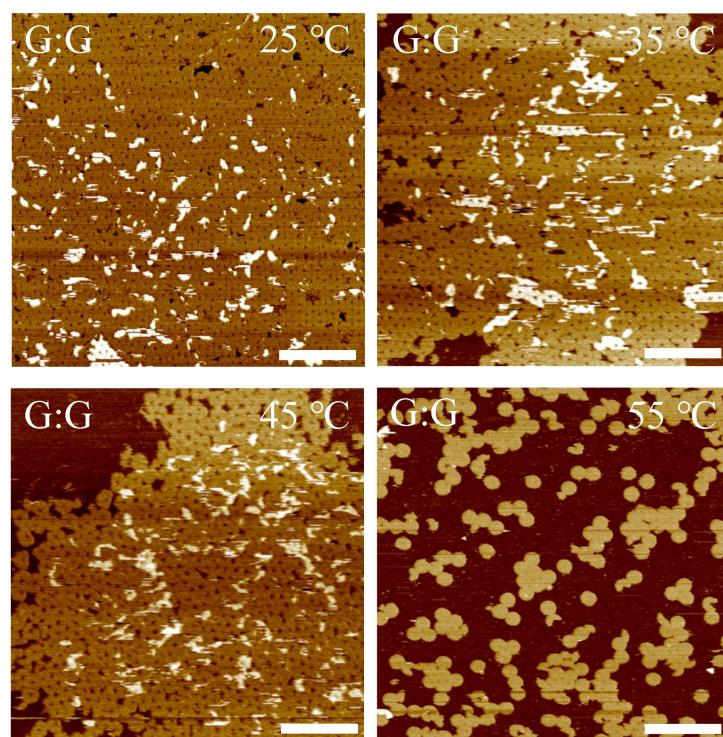


Fig. S4 Representative AFM images of G:G-mediated DNA origami assemblies after incubation at 25 °C, 35 °C, 45 °C, and 55 °C for 30 min. Scale bar: 600 nm.

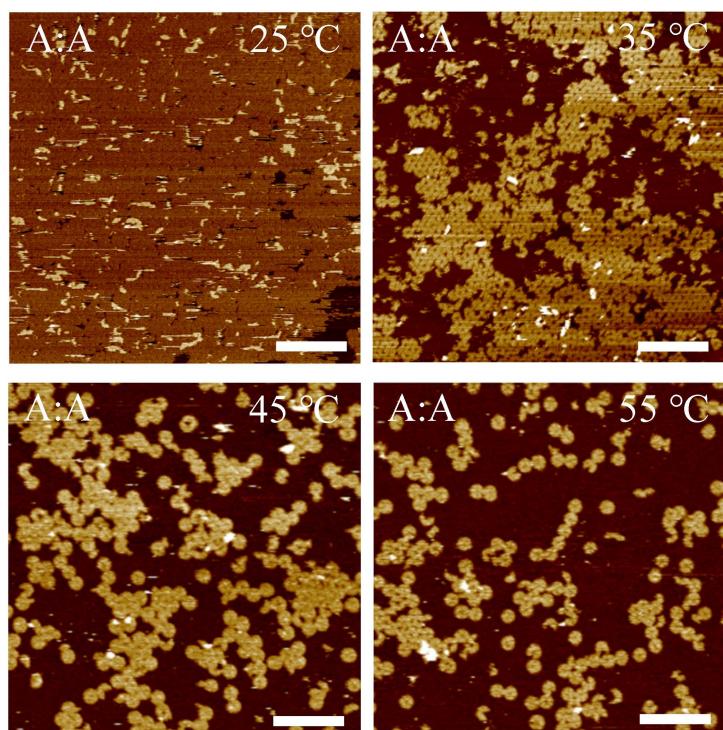


Fig. S5 Representative AFM images of A:A-mediated DNA origami assemblies after incubation at 25 °C, 35 °C, 45 °C, and 55 °C for 30 min. Scale bar: 600 nm.

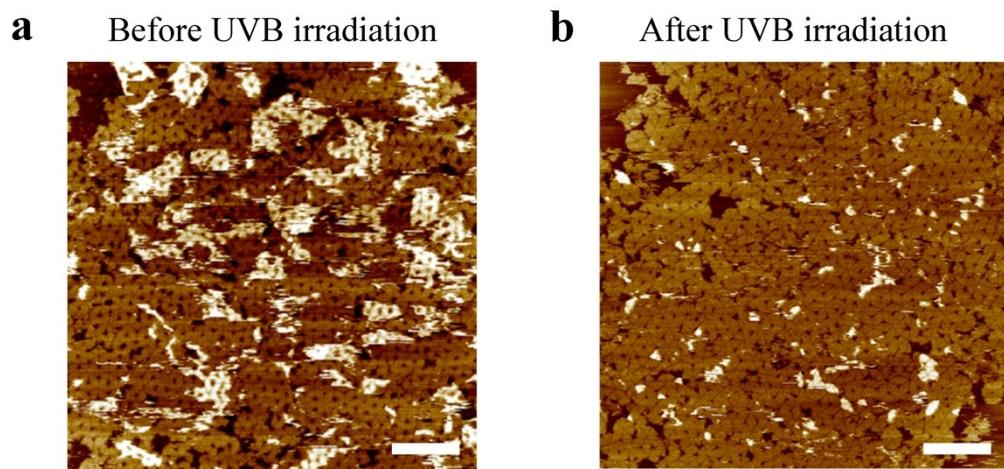


Fig. S6 (a) Representative AFM images of DNA origami large-scale assemblies by A:A recognition before UVB irradiation. (b) Representative AFM images of DNA origami large-scale assemblies by A:A recognition after UVB irradiation. Scale bar: 600 nm.

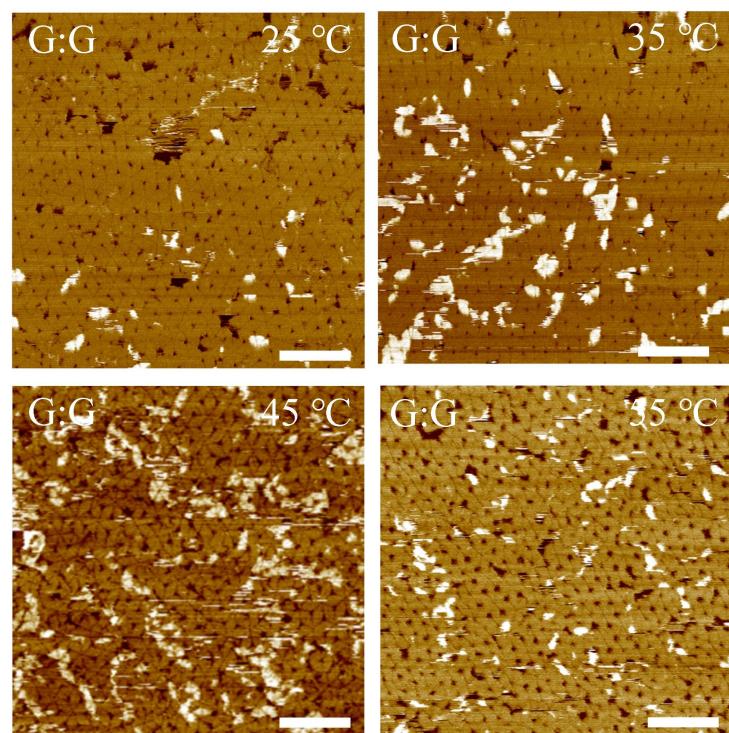


Fig. S7 Representative AFM images of DNA origami assemblies mediated by G:G recognition after UVB irradiation for 10 min and thermal incubation at 25 °C, 35 °C, 45 °C, and 55 °C for 30 min. Scale bar: 300 nm.

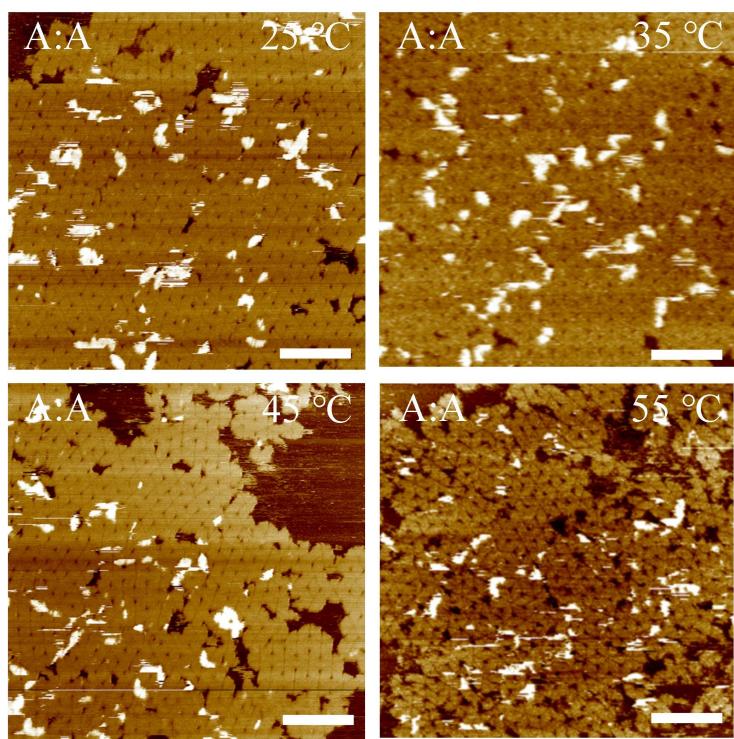


Fig. S8 Representative AFM images of DNA origami assemblies mediated by A:A recognition after UVB irradiation for 10 min and thermal incubation at 25 °C, 35 °C, 45 °C, and 55 °C for 30 min. Scale bar: 300 nm.

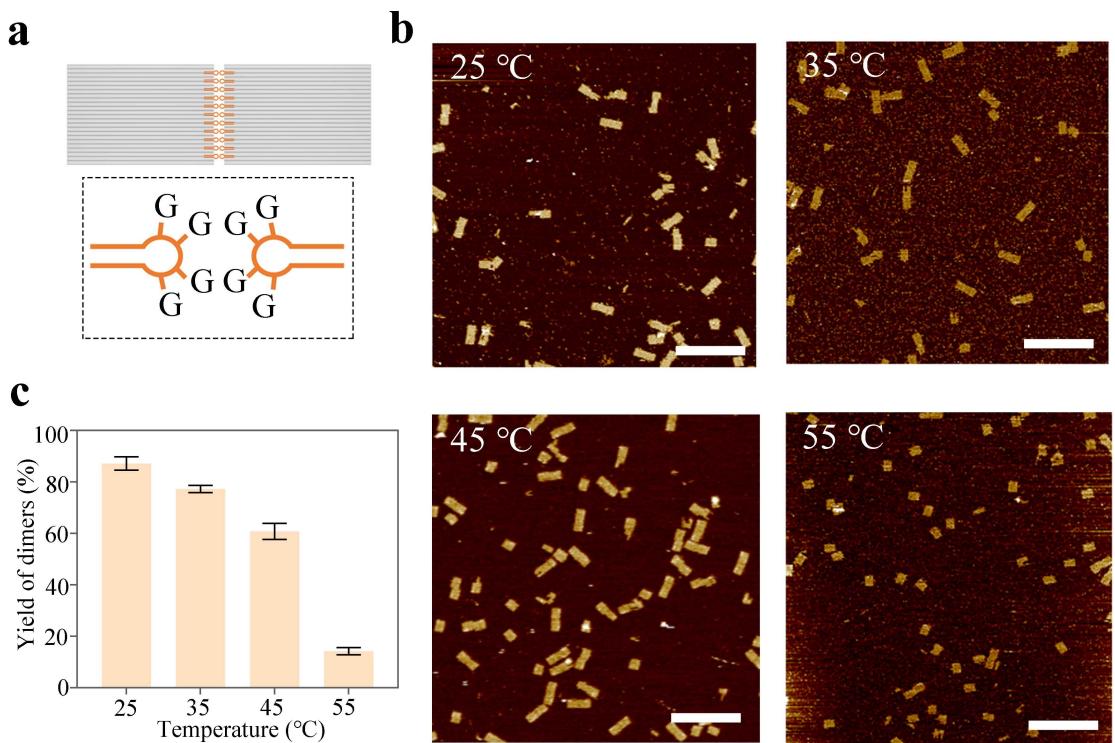


Fig. S9 (a) Schematic illustration of force-driven G:G base recognition-mediated origami dimerization. (b) Representative AFM images of origami dimers mediated by 4-nt polyG loop recognition at 25 °C, 35 °C, 45 °C and 55 °C, respectively. Scale bars: 500 nm. (c) Histogram showing the yield of rectangular origami dimers at 25 °C, 35°C, 45°C and 55°C analyzed from AFM images, respectively ($n=197, 212, 179, 191$).

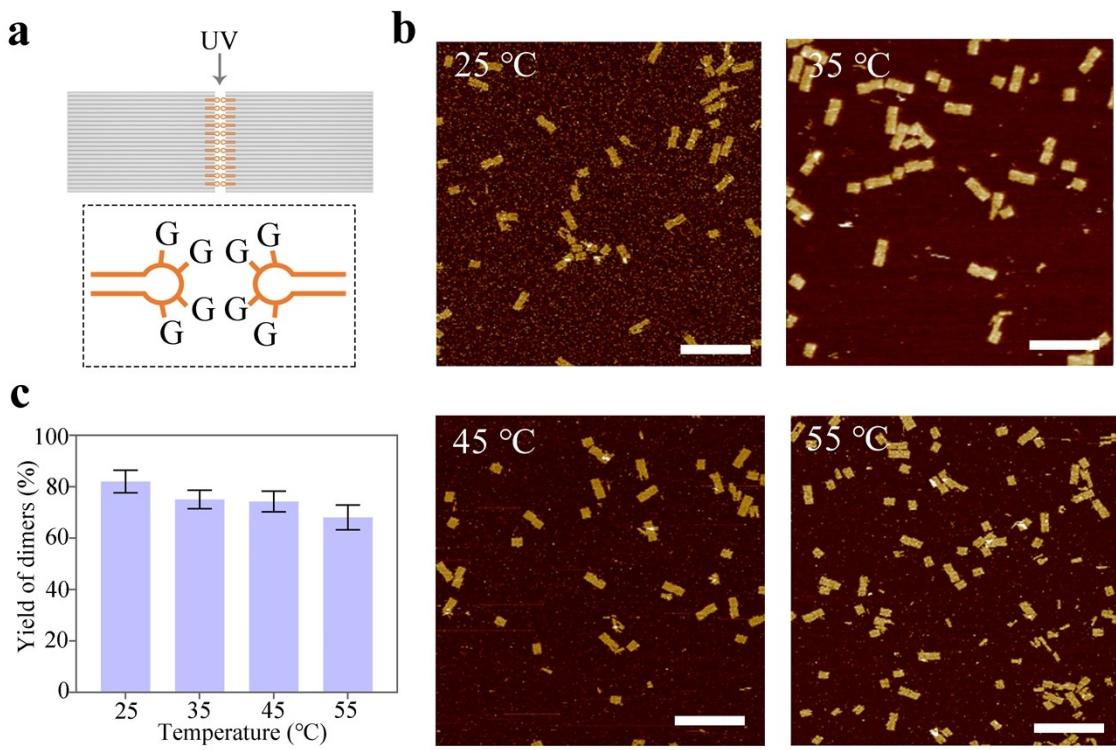


Fig. S10 (a) Schematic illustration of force-driven G:G base recognition-mediated origami dimerization after UVB pre-treatment. (b) Representative AFM images of origami dimers mediated by 4-nt loopG recognition. The samples were analysed after 10 min UVB irradiation followed by 30 min incubation at 25 °C, 35 °C, 45 °C, and 55 °C. Scale bars: 500 nm. (c) Histogram showing the yield of rectangular origami dimers at 25 °C, 35 °C, 45 °C and 55 °C after UVB pre-treatment analyzed from AFM images, respectively ($n=177, 169, 182, 188$).

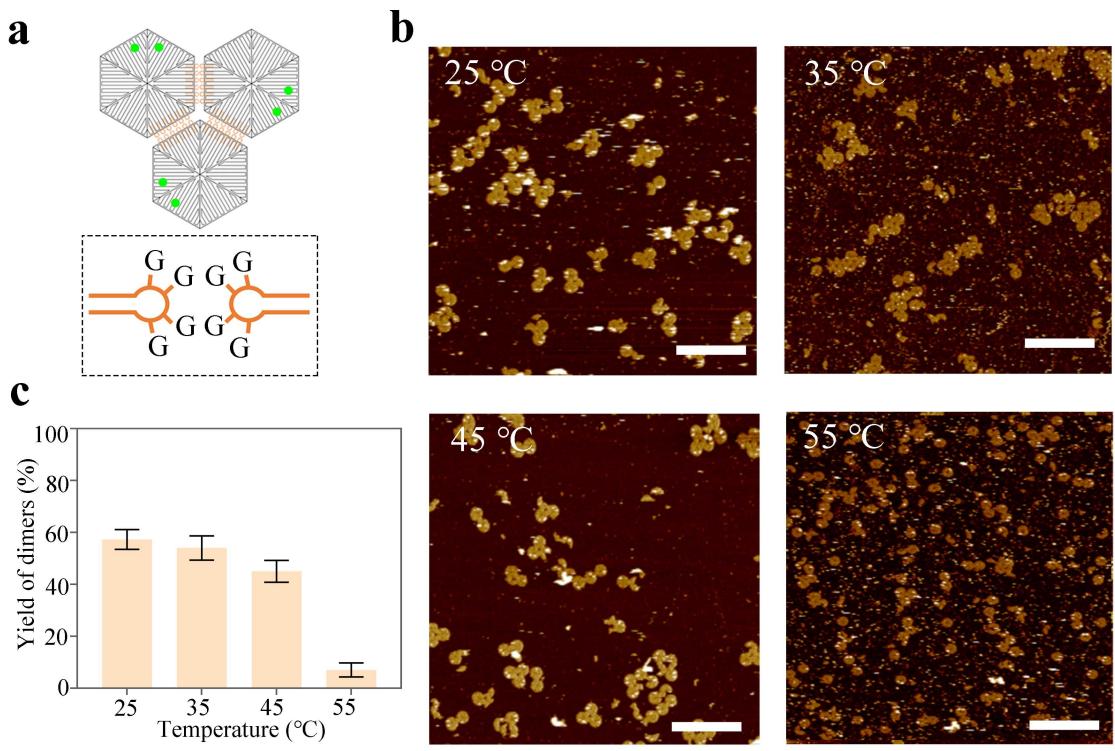


Fig. S11 (a) Schematic illustration of force-driven G:G base recognition-mediated origami trimerization. (b) Representative AFM images of origami trimers mediated by 4-nt polyG loop recognition at 25 °C, 35 °C, 45 °C and 55 °C, respectively. Scale bars: 600 nm. (c) Histogram showing the yield of rectangular origami trimers at 25 °C, 35 °C, 45 °C and 55 °C analyzed from AFM images, respectively ($n= 179, 162, 169, 172$, respectively).

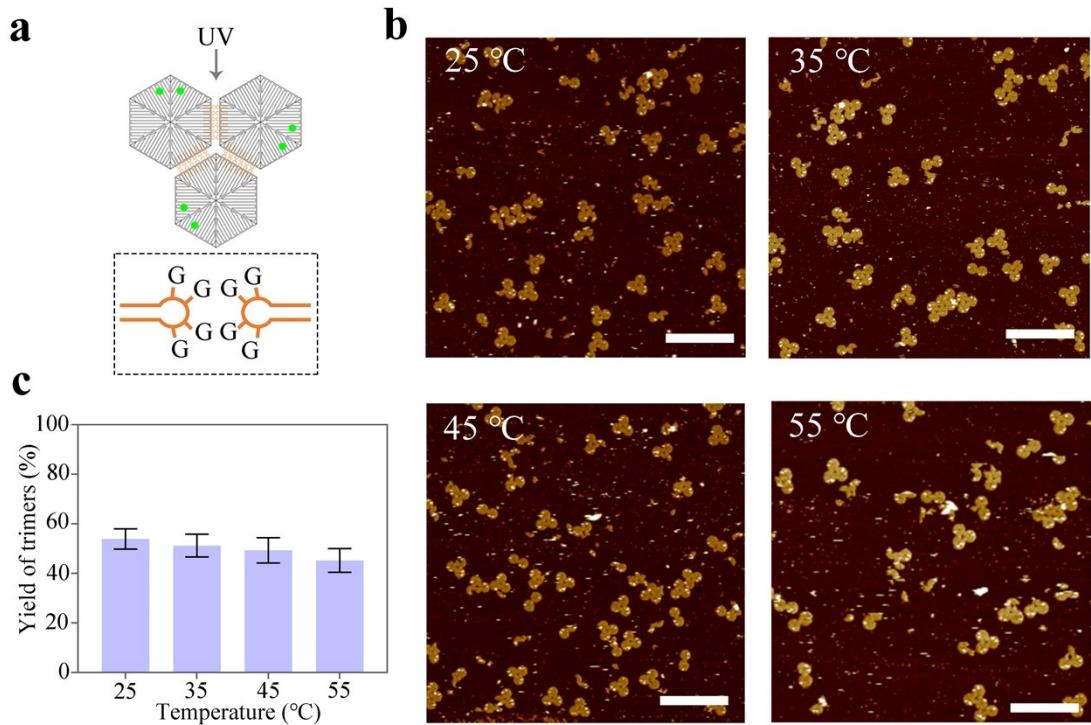


Fig. S12 (a) Schematic illustration of force-driven G:G base recognition-mediated origami trimerization after UVB pre-treatment. (b) Representative AFM images of the UVB irradiation effects on the thermostability of origami trimers mediated by 4-nt loopG. The samples were analysed after 10 min UVB irradiation followed by 30 min incubation at 25 °C, 35 °C, 45 °C, and 55 °C. Scale bars: 500 nm. (c) Histogram showing the yield of rectangular origami trimers at 25 °C, 35 °C, 45 °C and 55 °C after UVB pre-treatment analyzed from AFM images, respectively ($n=179, 166, 172, 180$, respectively).

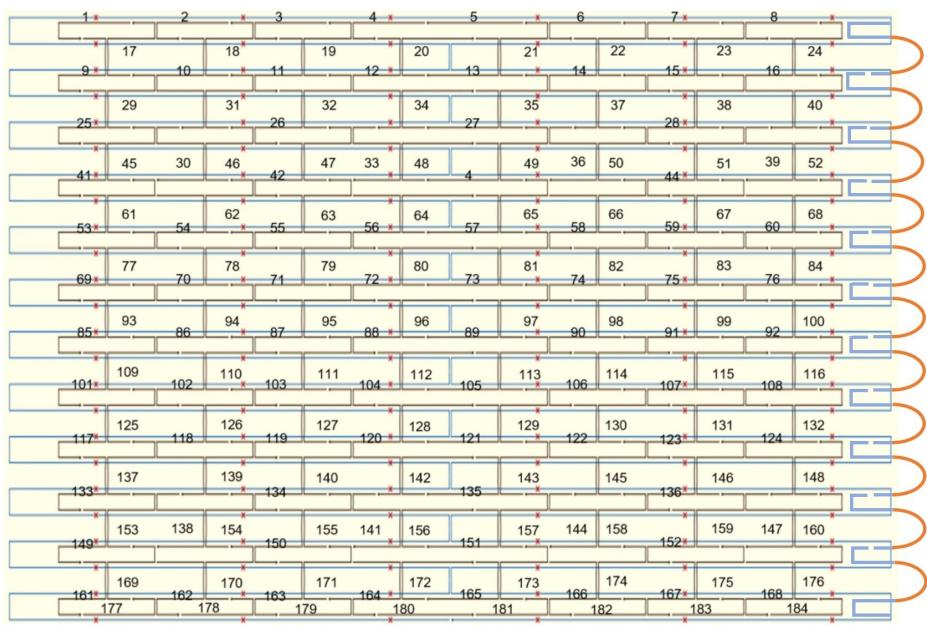


Fig. S13 Schematic representation of rectangular DNA origami with active edge staple designs.

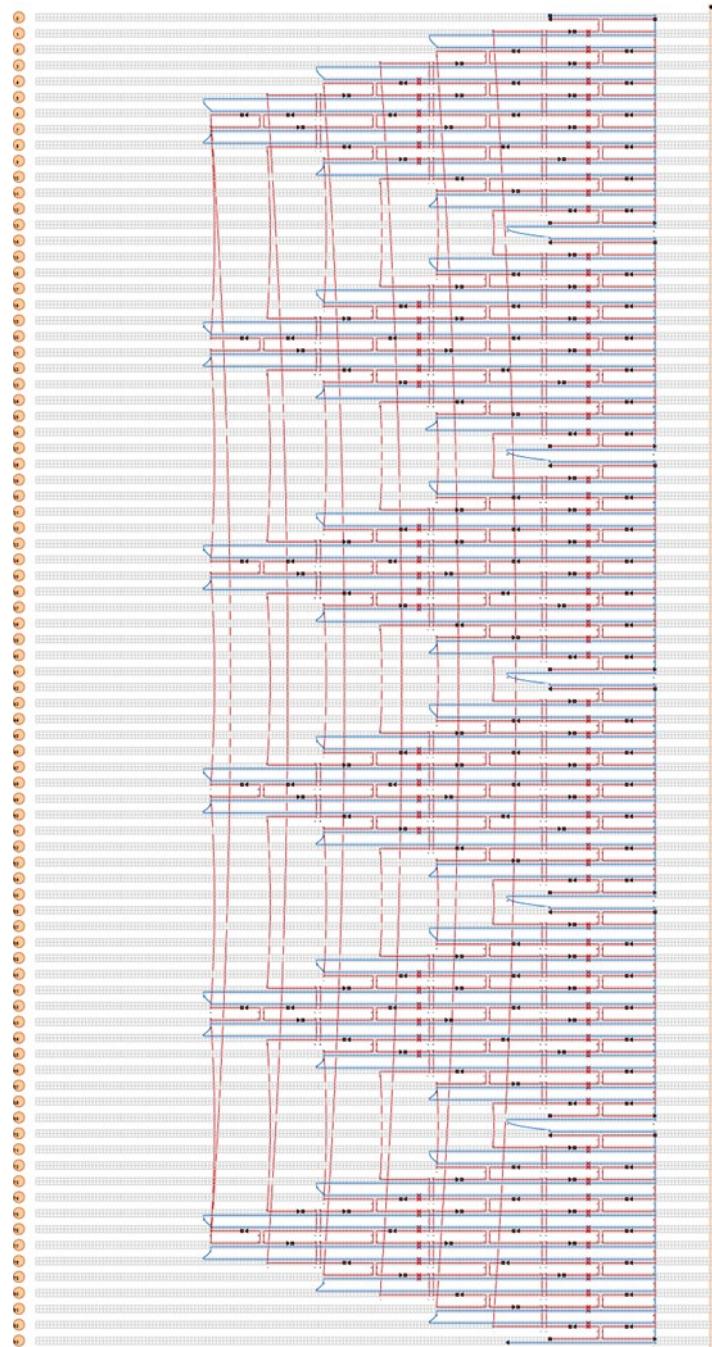


Fig. S14 Cadnano diagram of the hexagonal DNA origami nanostructure.

Supplementary DNA Sequences

DNA sequences of rectangular origami

Core staples

Seq name	Sequence 5'-3'
R01	AGAAAGGAACAACTAAAGGAATTCAAAAAAAA
R02	ACAACTTCAACAGTTCAGCGGATGTATCGG
R03	TAAATGAATTTCTGTATGGGATTAATTCTT
R04	TCTAAAGTTGTCGTCTTCCAGCCGACAA
R05	TCCACAGACAGCCCTCATAGTTAGCGTAACGA
R06	TCACCAGTACAAACTACAACGCCTAGTACCAAG
R07	AGGAACCCATGTACCGTAACACTTGATATAA
R08	CCACCCTCATTTCAGGGATAGCAACCGTACT
R09	AGGCTCCAGAGGCTTGAGGGACACGGGTAA
R10	TTTATCAGGACAGCATCGGAACGACACCAACCTAAAACGAGGTCAATC
R11	AAACAGCTTTGCGGGATCGTCAACACTAAA
R12	TGACAACTCGCTGAGGCTTGATTATACCAAGCGCGATGATAAA
R13	TTAGGATTGGCTGAGACTCCTCAATAACCGAT
R14	GCGGATAACCTATTATTCTGAAACAGACGATTGGCCTTGAAGA
R15	GCGGATAACCTATTATTCTGAAACAGACGATTGGCCTTGAAGA
R16	GCCAC
R17	ACCAG
R18	GTATAGCAAACAGTTAATGCCAATCCTCA
R19	CAGGAGGTGGGTCAGTGCCTTGAGTCTCTGAATTACCGGGAA
R20	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R21	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R22	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R23	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R24	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R25	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R26	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R27	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R28	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R29	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R30	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R31	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R32	ACCGCTACAAAGGAGCCTTAATGTGAGAAT
R33	ACCGCTACAAAGGAGCCTTAATGTGAGAAT

R34	TCATCGCCAACAAAGTACAACGGACGCCAGCA
R35	CACCAGAAAGGTTGAGGCAGGTATGAAAG
R36	CACCCCTCAGAAACCATCGATAGCATTGAGCCATTGGAA
R37	CCACCCCTCTATTACAAACAAATACCTGCCTA
R38	GCCTCCCTCAGAATGGAAAGCGCAGTAACAGT
R39	AGCCACCACTGTAGCGCTTTCAAGGGAGGGAAGGTAAA
R40	AAATCACCTTCCAGTAAGCGTCAGTAATAA
R41	CATCAAGTAAAACGAACTAACGAGTTGAGA
R42	TCATTAGATGCGATTTAAGAACAGGCATAG
R43	GCAAGGCCTCACCAAGTAGCACCATTGGCTTGA
R44	TCAAGTTCATTAAGGTGAATATAAAAGA
R45	TACGTTAAAGTAATCTTGACAAGAACCGAACT
R46	TTATACCACCAAATCAACGTAACGAACGAG
R47	ATTACCTTGAATAAGGCTGCCAAATCCGC
R48	GATGGTTGAACGAGTAGTAAATTACCATTA
R49	CAGCAAAAGGAAACGTCACCAATGAGCCGC
R50	TCACCGACGCACCGTAATCAGTAGCAGAACCG
R51	GAAATTATTGCCTTACCGTCAGACCGGAACC
R52	ACCGATTGTCGGCATTTCGGTCATAATCA
R53	TTTAGGACAAATGCTTAAACAATCAGGTC
R54	ATGCAGATACATAACGGGAATCGTCATAAATAAGCAAAG
R55	TAAGAGCAAATGTTAGACTGGATAGGAAGCC
R56	CGTTTACCAAGACGACAAAGAAGTTTGCCATAATTGCA
R57	TTATTACGAAGAACTGGCATGATTGCGAGAGG
R58	CGTAGAAAATACATACCGAGGAAACGCAATAAGAACCGCA
R59	AACGCAAAGATAGCCAACAAACCCCTGAAC
R60	GTTTATTTGTCACAATCTTACCGAACGCCCTTAATATCA
R61	ATCCCCCTATACCACTTCAACTAGAAAAATC
R62	AATACTGCCAAAAGGAATTACGTGGCTCA
R63	AATAGTAAACACTATCATAACCCCTCATTGTGA
R64	CTTTGCAGATAAAAACCAAAATAAGACTCC
R65	ATACCCAACAGTATGTTAGCAAATTAGAGC
R66	AAGGAAACATAAAGGTGGCAACATTATCACCG
R67	AAGTAAGCAGACACCACCGAATAATATTGACG
R68	AATAGCTATCAATAGAAAATTCAACATTCA
R69	TTTACCCCAACATGTTAAATTCCATAT
R70	CGGATTGCAGAGCTTAATTGCTGAAACGAGTA
R71	CGAAAGACTTGATAAGAGGTATTTCGCA
R72	GCTTCAATCAGGATTAGAGAGTTATTTCA
R73	AGAGAGAAAAAAATGAAAATAGCAAGCAAAC
R74	TTAGACGGCCAAATAAGAAACGATAGAAGGCT
R75	AAAGTCACAAAATAACAGCCAGCGTTTA
R76	GAGAGATAGAGCGTCTTCCAGAGGTTTGAA

R77	CTGTAGCTTGAECTATTATAGTCAGTCATTGA
R78	GATGGCTTATCAAAAAGATTAAGAGCGTCC
R79	TTGCTCCTTCAAATATCGCGTTGAGGGGGT
R80	CCAACAGGAGCGAACCGAGACCAGCCTTAC
R81	TTAACGTCTAACATAAAACAGGTAACGGA
R82	ATCCCAATGAGAATTAACTGAACAGTTACAG
R83	GCCAGTTAGAGGGTAATTGAGCGCTTAAGAA
R84	ACGCTAACACCCACAAGAATTGAAAATAGC
R85	AACAGTTTGTACCAAAACATTTATTTC
R86	GATTAGTCATAAAGCCTCAGAGAACCCCTCA
R87	AATGGTCAACAGGCAAGGCAAAGAGTAATGTG
R88	TTGGGGATAGTAGTAGCATAAAAGGCCG
R89	CCAATAGCTCATCGTAGGAATCATGGCATCAA
R90	TATCCGGTCTCATCGAGAACAGCGACAAAAG
R91	GCGAACCTCCAAGAACGGGTATGACAATAA
R92	GCCTTAAACCAATCAATAATCGGCACGCGCCT
R93	TAAATCGGGATTCCAATTCTGCGATAATG
R94	AAATTAAAGTTGACCATTAGATACTTTGCG
R95	TAAATCATATAACCTGTTAGCTAACCTTAA
R96	TTCTACTACCGAGCTGAAAAGGTTACCGCGC
R97	TTTATTAAAGCAAATCAGATATTTTGT
R98	GTACCGCAATTCTAACGACGCGAGTATTATT
R99	CTTATCATTCCCAGCTGCGGGAGCCTAATT
R100	TGTAGAAATCAAGATTAGTTGCTCTTACCA
R101	AACGCAAATCGATGAACGGTACCGGTTGA
R102	TATATTGTCATTGCCTGAGAGTGGAAAGATT
F103	TAGGTAAACTATTTGAGAGATCAAACGTTA
R104	GAGACAGCTAGCTGATAAATTAAATTGT
R105	GTAATAAGTTAGGCAGAGGCATTATGATATT
R106	GTAAAGTAATGCCATATTAAACAAACTTT
R107	ACAACATGCCAACGCTAACAGTCTTCTGA
R108	GTTTATCAATATCGTTATACAAACCGACCGT
R109	AACAAGAGGGATAAAAATTAGCATAAAGC
R110	GCTATCAGAAATGCAATGCCTGAATTAGCA
R111	GAGGGTAGGATTCAAAAGGGTGAGACATCCAA
R112	CAACCGTTCAAATCACCATCAATTGAGCCA
R113	CATGTAATAGAATATAAAGTACCAAGCCGT
R114	AATTGAGAATTCTGTCCAGACGACTAACCAA
R115	AGTATAAAGTTAGCTAATGCAGATGTCTTC
R116	TTAGTATCACAATAGATAAGTCCACGAGCA
R117	TAATCAGCGGATTGACCGTAATCGTAACCG
R118	GTATAAGCCAACCGTCGGATTCTGACGACAGTATCGGCCGCA AGGCG

R119	ATATTTGGCTTCATCAACATTATCCAGCCA
R120	TAAATCAAAATAATTGCGCTCGGAAACCAGGCAAAGGGAAGG
R121	ATCGCAAGTATGTAAATGCTGATGATAGGAAC
R122	TCAAATATAACCTCCGGCTAGGTAAACAATTTCATTGAAGGCGAATT
R123	CCTAAATCAAAATCATAGGTCTAACAGTA
R124	GTGATAAAAAGACGCTGAGAAGAGATAACCTGCTCTGTTCGGGAGA
R125	ACAAACGGAAAAGCCCCAAAAACACTGGAGCA
R126	GCGAGTAAAATATTAAATTGTTACAAAG
R127	TGTAGCCATTAAAATTGCGATTAAATGCCCGA
R128	GCCATCAAGCTCATTAAACCACAAATCCA
R129	TATAACTAACAAAGAACGCGAGAACGCCAA
R130	ACCTTTTATTAGTTAATTCTAGGGCTT
R131	GAATTTATTAAATGGTTGAAATATTCTTACC
R132	CTTAGATTAAAGCGTTAAATAAAGCCTGT
R133	TGCATCTTCCCAGTCACGACGGCCTGCAG
R134	GCTTCCGATTACGCCAGCTGGCGGCTTTCTG
R135	AGAAAACAAAGAACGATGATGAAACAGGCTGCG
R136	CATAAAATCTTGAAATACCAAGTGTAGAAC
R137	CCAGGGTTGCCAGTTGAGGGGACCCGTGGGA
R138	ATTAAGTTACCGAGCTCGAATTGGAAACCTGTCGTGC
R139	GATGTGCTTCAGGAAGATCGCACAAATGTGA
R140	TCTTCGCTGCACCGCTTCTGGTGCGGCCTTCC
R141	GCGATCGGCAATTCCACACAAACAGGTGCCTAATGAGTG
R142	CAACTGTTGCCATTGCCATTCAAACATCA
R143	CTGAGCAAAATTAATTACATTGGGTTA
R144	ATTCAATTGGATTATACTAAGAAACCACCAAGAAC
R145	CGCGCAGATTACCTTTTAATGGGAGAGACT
R146	CCTGATTGCAATATATGTGAGTGTAGCAATAGT
R147	AACAATAACGTAAAACAGAAATAAAATCCTTGCCCGAA
R148	CTTTACAAAATCGTCGCTATTAGCGATAG
R149	GTCGACTTCGGCCAACGCCGGGTTTTC
R150	CTGTGTGATTGCGTTGCGCTCACTAGAGTTGC
R151	GCAATTCACATATTCTGATTATCAAAGTGTAA
R152	CTACCATAGTTGAGTAACATTAAAATAT
R153	TTAATGAACTAGAGGATCCCCGGGGGTAACG
R154	TTCCAGTCGAATCATGGTCATAAAAGGGG
R155	CACATTAAAATTGTTATCCGCTCATGCC
R156	AAGCCTGGTACGAGGCCGAAGCATAGATGATG
R157	ATTATCATTCAATATAATTCTGACAATTAC
R158	GCGAACATCTGAATAATGGAAGGTACAAAT

R159	ATTTAAAATCAAAATTATTGCACGGATTG
R160	CTCGTATTAGAAATTGCGTAGATACTAC
R161	TTTCACTCAAAGGGCGAAAAACCACCA
R162	AGCTGATTGCCCTCAGAGTCCACTATTAAAGGGTGCCT
R163	AGCAAGCGTAGGGTTGAGTGTAGGGAGCC
R164	CCCAGCAGGCGAAAAATCCCTATAAATCAAGCCGGCG
R165	TCAATATCGAACCTCAAATATCAATTCCGAAA
R166	TCAACAGTTGAAAGGAGCAAATGAAAAATCTAGAGATAGA
R167	CTTAGGGCCTGCAACAGTGCCAATACGTG
R168	AGATTAGAGCCGTCAAAAAACAGAGGTGAGGCCTATTAGT
R169	CTCCAACGCAGTGAGACGGCAACCAGCTGCA
R170	TGGAACAACCGCCTGGCCCTGAGGCCCGCT
R171	GCCGAGAGTCCACGCTGGTTGCAGCTAACT
R172	TCGGCAAATCCTGTTGATGGTGGACCCTCAA
R173	ACCTTGCTTGGTCAGTTGGCAAAGAGCGGA
R174	AGCCAGCAATTGAGGAAGGTTATCATCATT
R175	TTAACACCAGCACTAACAACTAACCGTTATT
R176	CAGAAGATTAGATAATACATTGTCGACAA
R177	CAAATCAAGTTTTGGGTCGAAACGTGGA
R178	AAAGCACTAAATCGGAACCCATAATCCAGTT
R179	CCCGATTAGAGCTGACGGGGAAAAAGAATA
R180	AACGTGGCGAGAAAGGAAGGGAAACCAGTAA
R181	TAAAAGGGACATTCTGGCCAACAAAGCATC
R182	ACCCTTCTGACCTGAAAGCGTAAGACGCTGAG
R183	GCACAGACAATATTTGAATGGGTCAGTA
R184	CTTAATGCGCGAACTGATAGCCCCACCAG

Right edge staples (4adenine-loop)

Seq name	Sequence 5'-3'
R185	CAGAACCGCCACCCCTC TCAGAACCC
R186-A	GCCACCCTAAAAATACAGGAGTGTACTGTACATGGC
R187-A	TTTGATGAAAACTGTTGCCATCTTCATAGCCCC
R188-A	CTTATTAGAAAACAAAGACAAAAGGGCGTATGGTT
R189-A	ACCAGCGCAAAAAGAGCAAGAACAAATGGTAAGCC
R190-A	CAATAATAAAAACAATTATCCTGAATATTTGCA
R191-A	CCCAGCTAAAAAATCCCCATCCTAACCTGAACAAAG
R192-A	AAAAATAA AAAACATAATTACTAGAAAAGAATAAAC
R193-A	ACCGGAATAAAAATCCTGAAAACATAATTAAATT
R194-A	TCCCTTAGAAAAAGATGAATATACAGTATTCAGGT
R195-A	TTAACGTCAAAAAGACTTACAAACAATAGGATT
R196-A	GAAGTATTAAAA AAAAATACCGAACGAACTAAACATGCCATT

Right edge staples (4guanine-loop)

Seq name	Sequence 5'-3'
R185	CAGAACGCCACCCCTC TCAGAAC
R186-G	GCCACCCT GGGG ATACAGGAGTGTACTG TACATGGC
R187-G	TTTGAT GGGGGG CGTTGCCATCTTTC ATAGCCCC
R188-G	CTTATTAG GGGG CAAAGACAAAAGGGCG TATGGTT
R189-G	ACCAGCGC GGGG GAGAGCAAGAAACAATG GTTAAGCC
R190-G	CAATAATA GGGG CAATTTATCCTGAAT ATTTGCA
R191-G	CCCAGCTA GGGG TATCCCATCCTAATT TGAAACAAG
R192-G	AAAAATAA GGGG CATAATTACTAGAAAA GAATAAAC
R193-G	ACCGAAT GGGG AATCCTGAAAACATA ATTAATT
R194-G	TCCCTTAG GGGG AGATGAATATACAGTA TTTCAGGT
R195-G	TTAACGTC GGGG AGACTTACAAACAAT AGGATT
R196-G	GAAGTATT GGGG AAAAATACCGAACGAA CTAAAACATGCCATT

Biotinylated sequences

Seq name	Sequence 5'-3'
BioR30	ATAAGGGAACCGGATATT CATTACGTCAGGACGTTGGAA-biotin
BioR33	TTGTGTCGTGACGAGAACACCAAATTCAACTTTAAT-biotin

DNA sequences of hexagonal origami

Core staples

Seq name	Sequence 5'-3'
HE01	CAGTACATAAGTAAATCGTCGCTATAAACTTT
HE02	CCCTTAATTACCTTTTAATAGTTACAAAATCGCGCGTCAGATG
HE03	GACCAGGCTTACTTAGCCGGAACGTAAAACAC
HE04	ATACAAAGAACTGGCATGATTTCACCGCTAACAGTAAGCCTGT
HE05	CTACAGAGAAGTACAACGGAGATTTCATAACCCCTCGTTAGAACACG
HE06	GCGAACACAGCTTGAGGACTAAACCGATATATT
HE07	ATTCAGAGGCTTTGCAAAAGCCACATTCAACTAATGAAATCTAAC
HE08	GAGAGATGGAGAATTAACTGAATTTCACCTCTAACCGCGCCT
HE09	ATAGCTTTTTAAACTATCGGCCTGGGCTA
HE10	GTAATGTGTAAATACCTTGCAGGGTAGCATT
HE11	GAATTAAAAGAAACGCAAACGAGGAAACGCAATATAATATCA
HE12	AAATATCACGGTCAGTATTAAACACGGGACATT
HE13	GATCGTCACCTTTATAGTCAGAACGACTAAA
HE14	TCATACATAAGTTAACGGGG

HE15	TCATCTTAGTTCCATTAAACGGCGACAATG
HE16	GCCGCTTAACTAAAGGAA
HE17	TTGCCAGAGGTCCAATACTGCGGAACCAGACCG
HE18	GACGATAAAAGGAATTACGAGGTTAATTGTGTCGAAATCACC AAGC
HE19	ACAGTGCAAAGCATCACCTGCTAGATAAT
HE20	CGTTAGACCGCTACAGGGCGCGTTGGCAACAGCTGATTGGTT GCG
HE21	ATATACCCGAAAGACTTCAATGCTTAAACAGTTCTACCAGAC
HE22	ATTTAGACATTATAATCAGTGAGGCAATCGTC
HE23	ACGAGTAGTAAATTGTTGTGAA
HE24	TTAATGCGATCAGAGCGGGAGCTATCTGTCCATCACGCAAAACG C
HE25	GAAGCAAAATTGCTCCTTGAGTTAGCT
HE26	ACAAAGTTAACGCCAATAATAAACATAAAAAACAGATATT TT
HE27	TTGCGTGCTAAACAACTTCTTCATTAGCAAGGCCGGTGAGCC AT
HE28	AAGAAACAATTAAAGAAAAGTAAGCAATAGAA
HE29	GCCACCCTGCCAATAGGAACCCATTGTCGTCTTCCAGAAAAAA A
HE30	TTATTTCAATCAATAATCGGCTGGACAATAA
HE31	AAGTTGTACCGTAACACTGAACCGTACTCAGGAGGTAGCGGG GT
HE32	GCTCCATGGCATAGGCTGGCTGATTGGACGTTGGAAAGAAC GATACA
HE33	TCGGCCAAATGAGTGAGCTAACTCACGACGGC
HE34	TTTATTTATATTAAATGCACATCAATA
HE35	TCCAATCGCAAATAAGGCGTTAAATAACGCCAAC
HE36	TGATATTAGGGTAGCTATT
HE37	CATTCGCATAATCATAACAGGAAAAAACAT
HE38	ACCCAAAAGGCTGCCCTGACG
HE39	AATCAAGATTAGTTGATCTTAC
HE40	TGGGATTTAATAATAATTTCAGCTGAGGCTGCAGGGAGCA ACGG
HE41	CAGTAGCGAATCAAAATCACCGGAGGCCAC
HE42	ATTAGACGAACCCACAAGAATTGAGTTACCAGAAGGAAACGAC AC
HE43	CGCCTGGCAAATCAAAAGAATAGTTGACGGGGAAAGCCGGCG CCGCGC
HE44	ATTATTCTTAACAATTTCATTGAGAATCCTTGAAAACAGCAA A
HE45	CCAATAGGGAGCGAGTAACAACCCTGAGGGGACGACGACCTC

	TT
HE46	ATCAGCTTACCGATAGTTGCGCGTAAAATA
HE47	GTAACAGTGCCGTACCTATTAA
HE48	TCAAATATTAATGGTTGAAATCGAGCCAG
HE49	GGTGCCTACGCGCGGGAGAGGCGCCCTTCAC
HE50	ACTCCAGCGCAACTGTTGGGAAGGGATCCCCGGGTACCGAGCAC AACAT
HE51	CATGAGGAGACCCCCAGCGATTATCGCGACCT
HE52	TCATGGAAATACAGAGATAGAACCCCTTAAAACAG
HE53	ATATTTATTCTACTAATAGTAGAGAAGCC
HE54	AGGTAAATTTATTTGTCAACAATCAGATAGCCGA
HE55	ATCAACATAAAATCAAAAATCTTCATCGAACGAGGGTAGTTAA AG
HE56	CCGAACGAATCAACAGTTGAAAGTTCAAACATCAAGAAAATT AAGACG
HE57	CCAGAAGGATGATGGCAATTCA
HE58	ATACCCAATAAAGGTGGCAACATAATCACC GT CACCGACTAAA CGTCA
HE59	ATAGCAACAGAACCGCCACCCTTACCGCCACCCTCAGAACCA GAG
HE60	AAATAAATCCGCCACCAGAACCACTTTGCCAT
HE61	AAGAGAACAGGAGGCCGATTAGCGTAACCACCCACCCGAACG TG
HE62	TAATAAGTTCTGTCCAGACGACTCTTCCT
HE63	GTTTATCATGCCATATTAAACAGAATAAACAC
HE64	TTAGGAGTCAATAGTGAATTCTAAACATC
HE65	ATTGAGAAACAATAGATAAGTCCTTAGGGTAATTGAGCGCATA ACGGA
HE66	CTGAGAAGTTGGTTATATAACTATCATAATTACTAGAAAAGGG CTTA
HE67	GTTAATAATGCGATTAAAGAACCTTTGACAAGAACCGGAGGT GTACA
HE68	ATTACATTTCAATTACCTGAGTTAAAATATCTTAGGCTGGT CA
HE69	CTGGCCAACCTACATTGACGCTCCACCGAGTAA
HE70	TGTGATAAGACAAAGAACCGCAGATAATTAAATT
HE71	TAGAAACCATCGTAGGAATCATTAAACAAATAAACAGCCGG AAGCGC
HE72	CATTTTGCAGCTCAAAGCGAATCGTCATAAAT
HE73	ACAGGAAGTAAAATAGCATGTCTTAGACAGTCAAATCACAT GCCTGA
HE74	AGAATGACAAAGATTAAGAGGAAGATGCTGTAGCTAACAAAT TCTGC

HE75	TTCTGAAAGTACCAGGC GGATAACGGAA TAGGTGTATCGTTTC
HE76	TATGACCCTAGGTAAAGATTCAATTGATAATCAGAAAAGTTT TTAA
HE77	GCCATGACAATATTTGAATCTGGTAAT
HE78	CCGCCGCGATTGGCCTTGATATAGTAAGCG
HE79	TAACGCCAAAAACCAAAATAGCGATTGAATCCCCCTCAAAATA TC
HE80	CCACCAACCACCATCGATAGCAGCCATTAAAGGT
HE81	TTAGTCTTAGAGAGTTACTACCTTTATATG
HE82	CGGAATATGTAATGCTGATTAGCGATAGCTTAGACAAAATTA
HE83	TTAGTATCTAACCTCCGGC
HE84	AAGGCTCCAAACATCGCCCACGCATAAGACTTTT
HE85	CGGTCCGTTGAAATCTCACGTTAGTAAATGAATTTCAGGG
HE86	TGATTGTTGGATTACATATCA
HE87	GTCACCACTAGCCCTCATAGTTAGCATCGGTTT
HE88	AGAGGGCGATCGGTGCGGGCAGTATCGGCCTCAGGATCAACAT
HE89	CCACGCTTGGTGGTCCGAAATAACAAGAG
HE90	TTGGGAATGTAGAAAATAC
HE91	GCGAGAAAGGAACCCCTAAAGGGATTGTTCCAGTTGGCGG CAAAA
HE92	GCTGCCAGCTTCCGGCACCTTTAACAGTTGATTCCCTGTTTA A
HE93	ACTAAATCGGAAGGGAAGAAAGCTAGCGGTACGCTGCAAGGG
HE94	GCGTTTAATTCGGATGGCTTAGAGCTATTAGATA
HE95	AATATACATGCACGTAAAACAGATTCATTTGCGGAACAAAAAA TCCTT
HE96	ACTACGTGAACCACATCGTAAAGC
HE97	TATCATTACATCGAGAACAAAGCAAGGCTTAT
HE98	CGCTATTACGCAGCTTGCATGCCTGCAAAGCCTGG
HE99	TGCCGAAAGATTAGAGCCGTCAATGAACCTC
HE100	TAAATGTAACGCCATAAAAATTAAATCGGTTGTACCAAGGC AAA
HE101	TTGCTCACATGAAAGTATTAAGTTGAATTACCGTTCCCTCAC AAAC
HE102	GAACGAGTAAAATTAAGCAATAATTCTGTAGCCAGCTTCAAG ATCGC
HE103	TCCCTTATCCTGAGAGAGTTGCAGTTAATGAA
HE104	CGTTATACAATTAGTATGTTAGCAAAGTAGAG
HE105	CAGTGCCACAGCTGGCGAAAGGGGCCGTGCATCTG
HE106	CCAGTGTGGATTCTCCGTGGTTAAATCAGCTCACCCAAA A
HE107	TGCGTTGGTCGTGCCAGCTGCACAAGCGGT
HE108	AGGTGAGGAACCCCTCAATCAATATAGCACTAA

HE109	CAACGCTATCCAATAAGAACGAGCCTTACAGAGAGAGAGC
HE110	TATTGGGCGAAGCATAAAGTAGGTGACTCT
HE111	CTTTCATACAGAACATCAAGTTGCAGGGAGGG
HE112	ACGAGCCGCCAGGGTGGTTTTGAGCACGTATAACGTAAT ACTTC
HE113	CGTAATGGCAAAAGAACATACACAGGCGCAG
HE114	CCAGCAAAATTTAGAACATAGAAAGGAACCGCG
HE115	AGCGTCATTGCAACAGGAAAATTAAACCCTGTAGCGCTTCCT
HE116	GTACGGTGTCTTCAGGCAAAGCGCCATTGGTC
HE117	AACATCCAAAATGGTCAATAACCTTAAGAGGT
HE118	ATATGCAAAAGCGGATTGC
HE119	CAACTAATCGTTATTAAATTAAATTTCAGGTTAACAGAG GCGA
HE120	ATCCAGAACGTAATAACATCACTTTCCGCTCACATTCCACTC GAATT
HE121	TCAGACTCCCCCTATTAGCGCACCAAGAG
HE122	TCCACTAAAAACCGTCTATCA
HE123	GGTAATCGATTGTATAAGCAAATATTGCATTAAATTGAACA
HE124	TTACCTAACGAACTAACGGAATGAGATTAGGAATAAGTT
HE125	AAGGCTATCAGGTAGATGAAC
HE126	TGAAATGCGACCAGTAATAAACGCCTGCA
HE127	TTTGATTACAATATTACCGCCAGCAAGAACATGTGGCACATAAA AATA
HE128	TATCCAAACGAGCGTCTTCCATTCAAATCAGATATAGAACG CGTT
HE129	ACAACAAACAGGAGCCTTAATTGTGTAACGATCTA
HE130	CCTCAGAGCCTCATTAAGCCAGTTAGAAGGATTAGGATTAA GTACC
HE131	AATTCACTATTCAACCGATTGACTTAGCG
HE132	ATGTAATTTCAGCTAATGCAGAACGAGCATG
HE133	AACGGCGGATATGGCGCATCGTAAGATGTGCT
HE134	ACGGTCAAGAGGACAGATGAACATTTCATT
HE135	CGTAATCATGCCATTCAAG
HE136	GAATTAGCAGATTAGTTGACCTAATTGCTGA
HE137	CCAATGAAGGAACCGCCTCCCTTTAGCCACCACCCCTATT CTGTA
HE138	AAATTATTGTAACAGTACCTTTTGCTTGAATACCAGGAAA
HE139	ACATTGTCGACAACCTCGTATTAGAAACCA
HE140	CCGGTATCGACTGCGGGAGGT
HE141	GCAAGGCTCACGACGTTGAAACATTAAT
HE142	CACGGAATAAGATTGACGGAAATTATTACCGTAAT
HE143	GTTGGCAAACCAACCAGCAGAACGACTGACCTGAA
HE144	ACAACATGTAGGCAGAGGCATTACCGACCG

Edge staples (4-guanine-loop)

Seq name	Sequence 5'-3'
GHE145	CCAACGTCAAAGGGCGTTAAAGAACGTGGACT GGGG CGAAAA TC
GHE146	CTGTTGAGGTTGCCCGAGCAGG GGGG TCCAGTCG
GHE147	GGAAACCTCGCTCACTGCCCGCTT GGGGGC CAGGGT
GHE148	TTTCCCAGGATTAAGTTGGTAAC GGGGGG TACGT
GHE149	TGGTGTAGTGACCGTAATGGGATA GGGG TTAATATT
GHE150	TTGTTAAAATTAAATTGTAAACG GGGG AGCAAACA
HE151	AGAGAATCTTGCCTGAGAGTCTGG

Edge staples (4adenine-loop)

Seq name	Sequence 5'-3'
AHE145	CCAACGTCAAAGGGCGTTAAAGAACGTGGACT AAAA CGAAAA TC
AHE146	CTGTTGAGGTTGCCCGAGCAGG AAA TCCAGTCG
AHE147	GGAAACCTCGCTCACTGCCCGCTT AAA GCCAGGGT
AHE148	TTTCCCAGGATTAAGTTGGTAAC AAA AGGTACGT
AHE149	TGGTGTAGTGACCGTAATGGGATA AAA TTAATATT
AHE150	TTGTTAAAATTAAATTGTAAACG AAA AGCAAACA
HE151	AGAGAATCTTGCCTGAGAGTCTGG

Biotinylated sequences

BioHE143	GTTGGCAAACCACCAAGCAGAAGACTGACCTGAA-biotin
BioHE12	AAATATCACGGTCAGTATTAACACGGGACATT-biotin
BioHE35	TCCAATCGCAAATAAGGCCTAAATAAACGCCAAC-biotin

References:

- 1 W. Fang, M. Xie, X. Hou, X. Liu, X. Zuo, J. Chao, L. Wang, C. Fan, H. Liu, and L. Wang, *J. Am. Chem. Soc.*, 2020, **142**, 8782-8789.