Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

DNA origami tubes with reconfigurable cross-sections

Anjelica Kucinic[1], Chao-Min Huang[2], Jingyuan Wang[2], Haijun Su[2], and Carlos E. Castro[2,3,]*

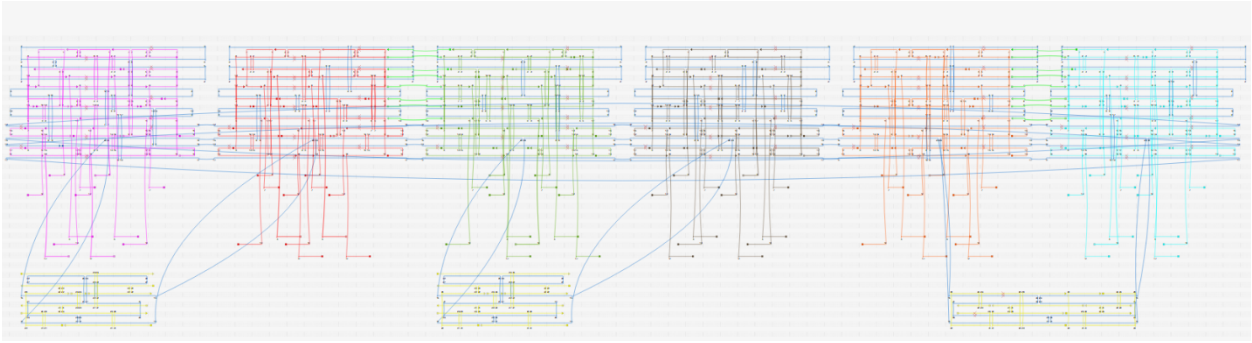
[1]Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus OH 43210

[2]Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus OH 43210

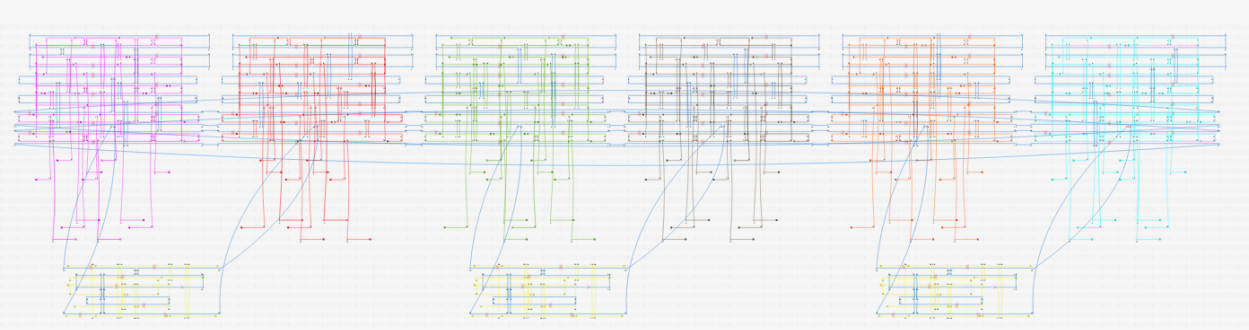
[3]Biophysics Graduate Program, The Ohio State University, Columbus OH 43210

[*]Corresponding author: castro.39@osu.edu

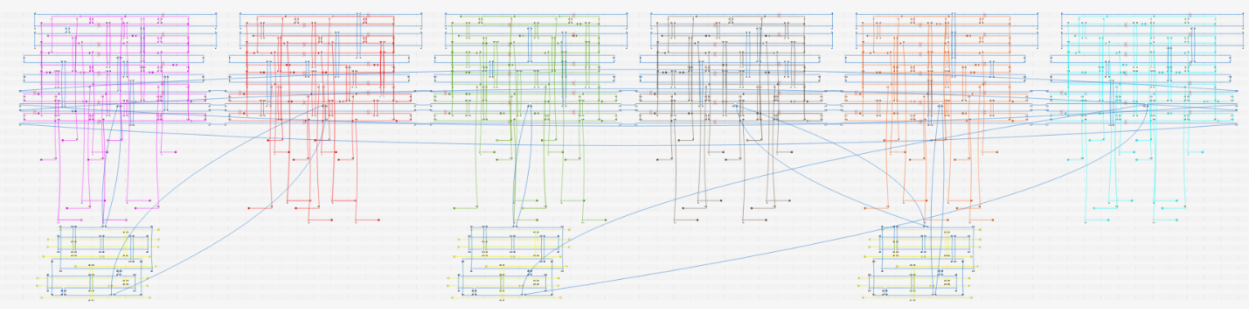
Table of Contents



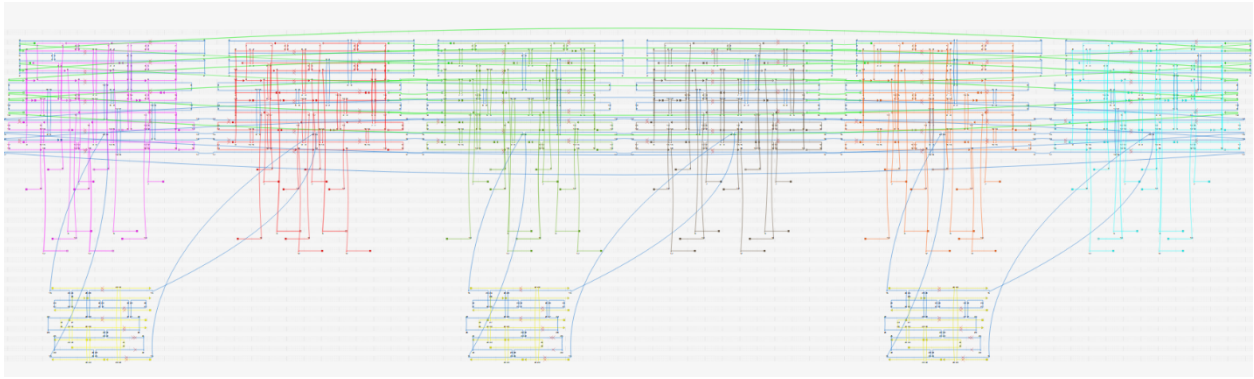
S.1: Rectangle scaffold and staple routing in cadnano[1]. Yellow staples correspond to strut regions and navy routing is scaffold.



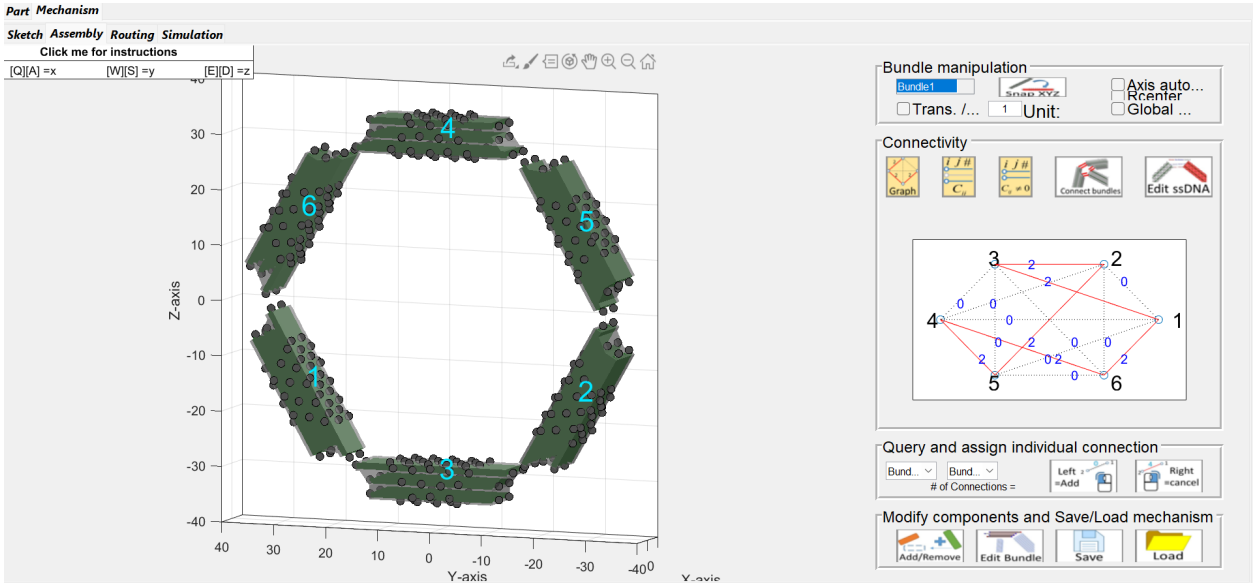
S.2: Hexagon scaffold and staple routing in cadnano[1]. Yellow staples correspond to strut regions and navy routing is scaffold.



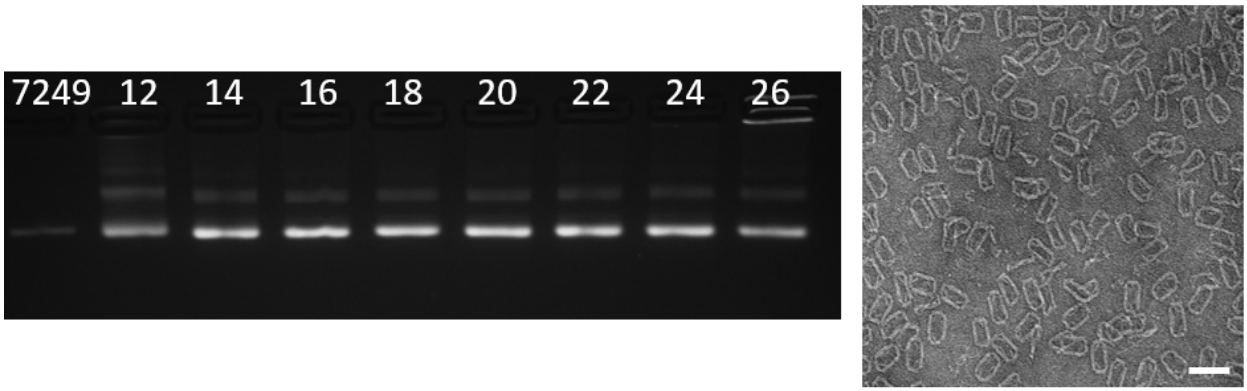
S.3: Flat closed scaffold and staple routing in cadnano[1]. Yellow staples correspond to strut regions and navy routing is scaffold.



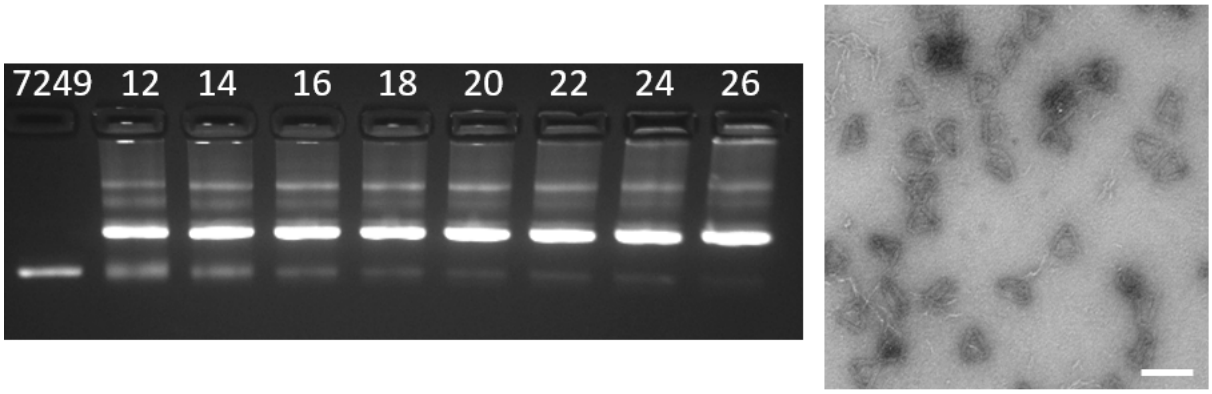
S.4: Flat closed scaffold and staple routing in cadnano[1]. Yellow staples correspond to strut regions and navy routing is scaffold.



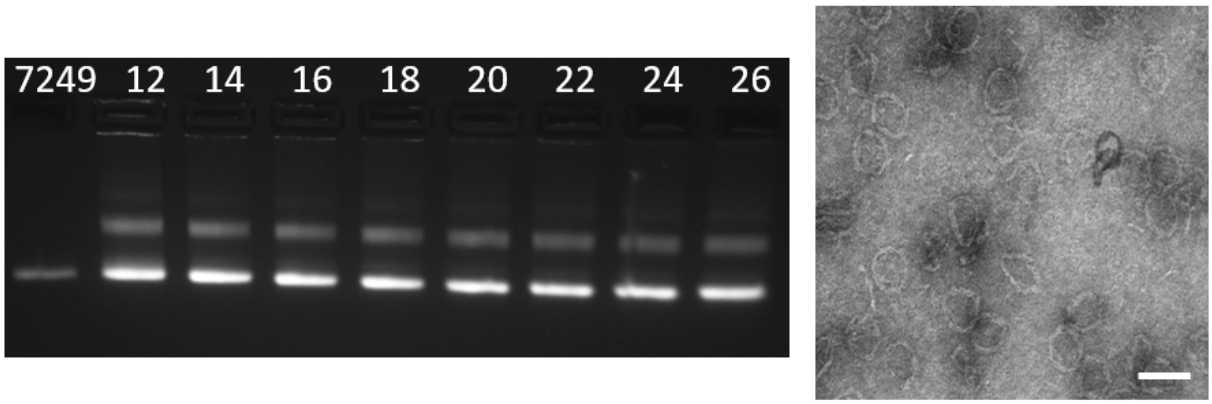
S.5: MagicDNA² screen capture of 6-bar mechanism with no strut or hinge connections. The bundles can be manipulated with strut additions to form 4 shapes.



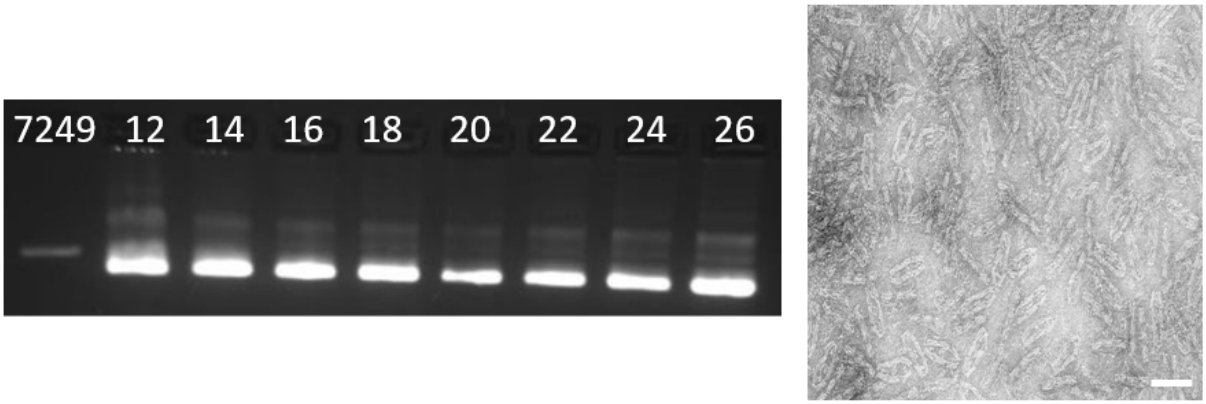
S.6: (top) agarose gel electrophoresis of rectangle with $MgCl_2$ [mM] salt gradient. (bottom) TEM image of well-folded rectangles at 20mM $MgCl_2$. Scale bar = 100nm.



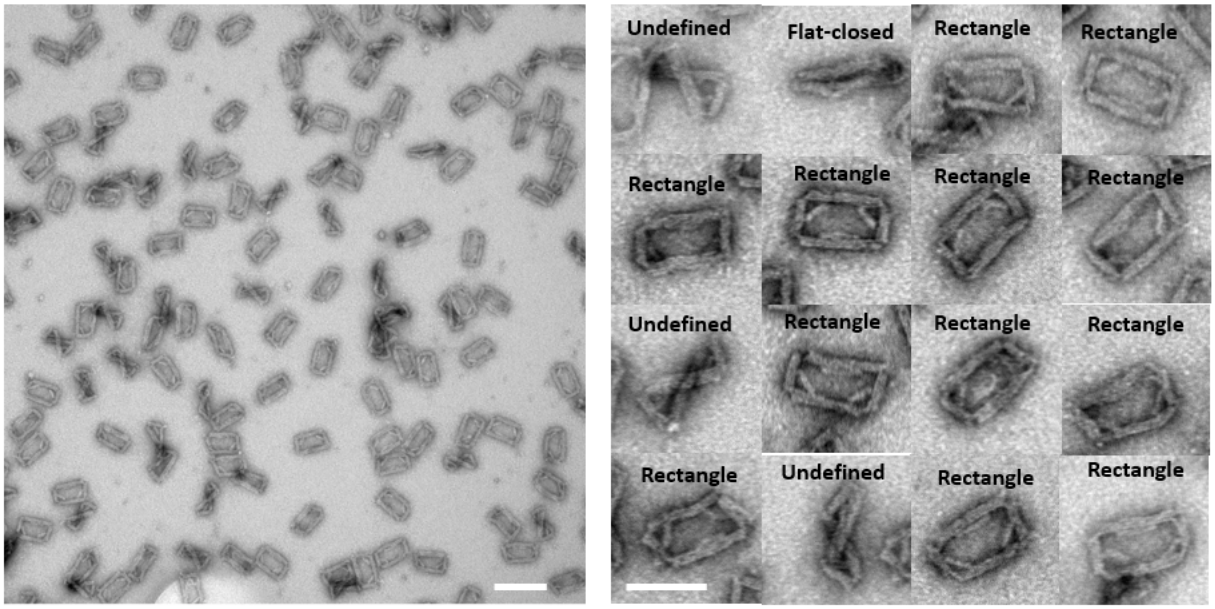
S.7: (top) agarose gel electrophoresis of triangle with $MgCl_2$ [mM] salt gradient. (bottom) TEM image of well-folded triangles at 12mM $MgCl_2$. scale bar = 100nm



S.8: (top) agarose gel electrophoresis of hexagon with $MgCl_2$ [mM] salt gradient. (bottom) TEM image of well-folded hexagons at 26mM $MgCl_2$. scale bar = 100nm



S.9: (top) agarose gel electrophoresis of flat closed with $MgCl_2$ [mM] salt gradient. (bottom) TEM image of well-folded flat closed shapes at 18mM $MgCl_2$. scale bar = 100nm



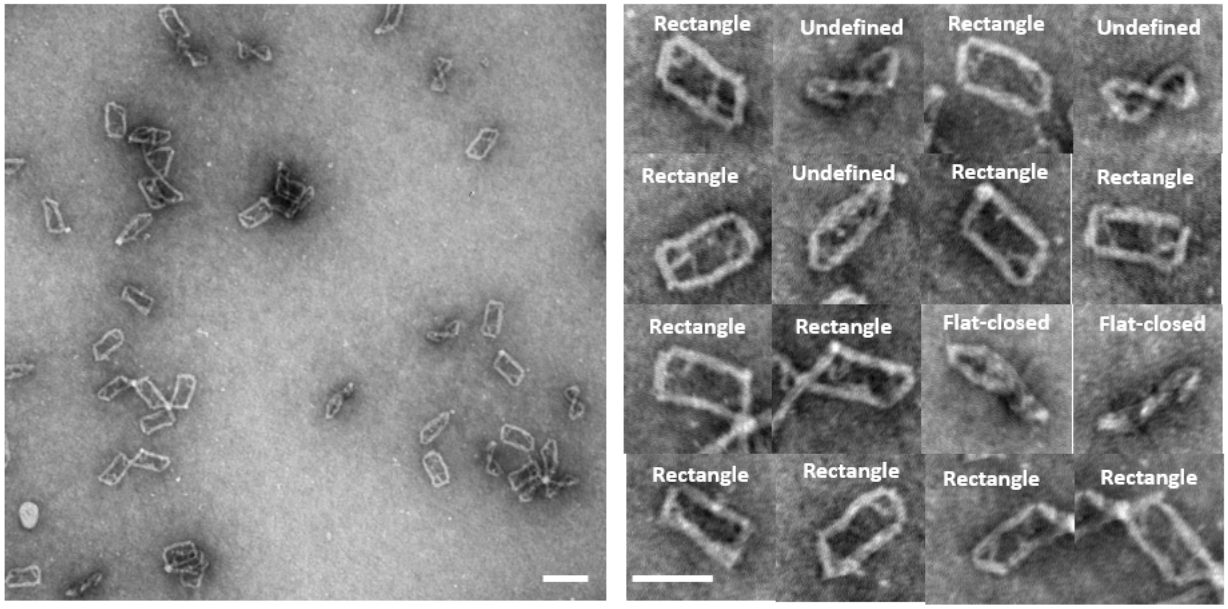
S.10: (Left) Zoom-out TEM image of long annealing ramp competitive folding reaction; (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)

Table 1: Free energy differences, sequence lengths, and oligo values for each shape

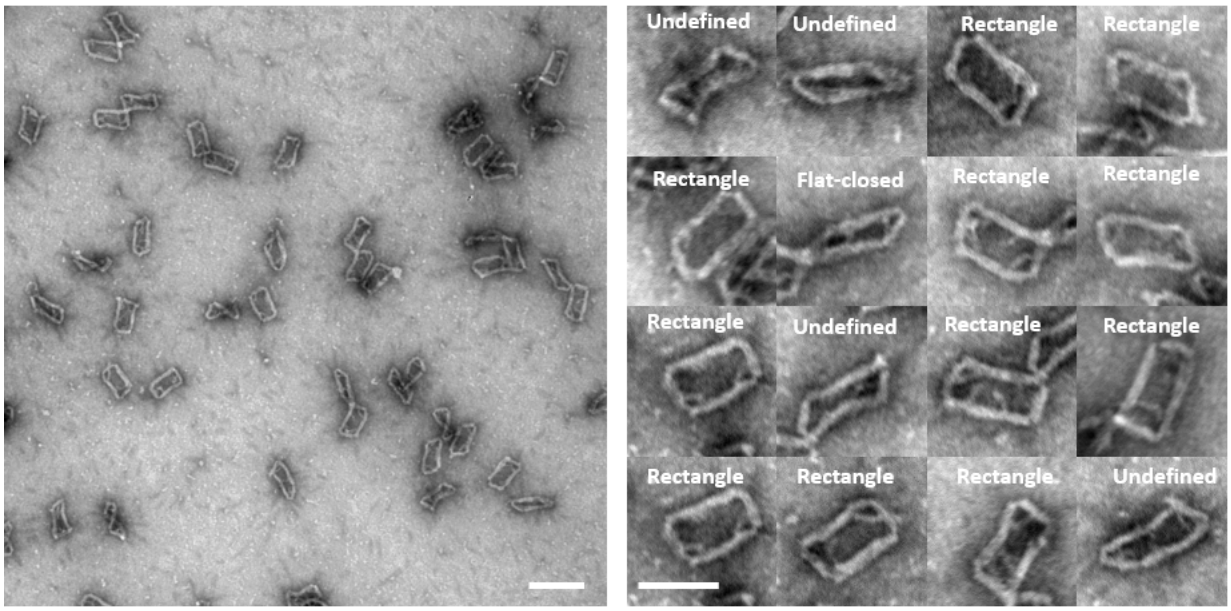
Shape	Free energy ΔG [kcal/mol]	# bases	# strut staples
Rectangle	-1377	1184*	31*
Hexagon	-1131	973	27
Flat Close	-1363	1203	29

* Includes fortifying staples

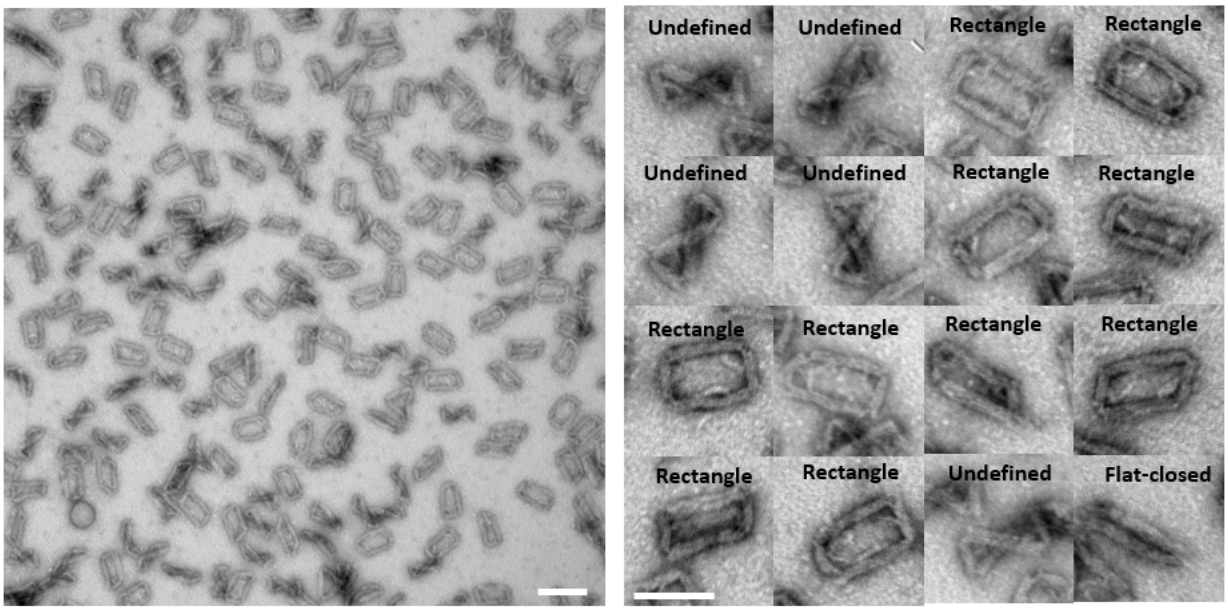
Table S1: Free energies of the strut staples for rectangle, hexagon and flat-closed. The free energy for the rectangle is calculated with the fortifying staples. Free energies are calculated using the nearest neighbor approximations[3–6] from a nearest neighbor calculator[7] with references describing improved nearest neighbor approximations[4–6].



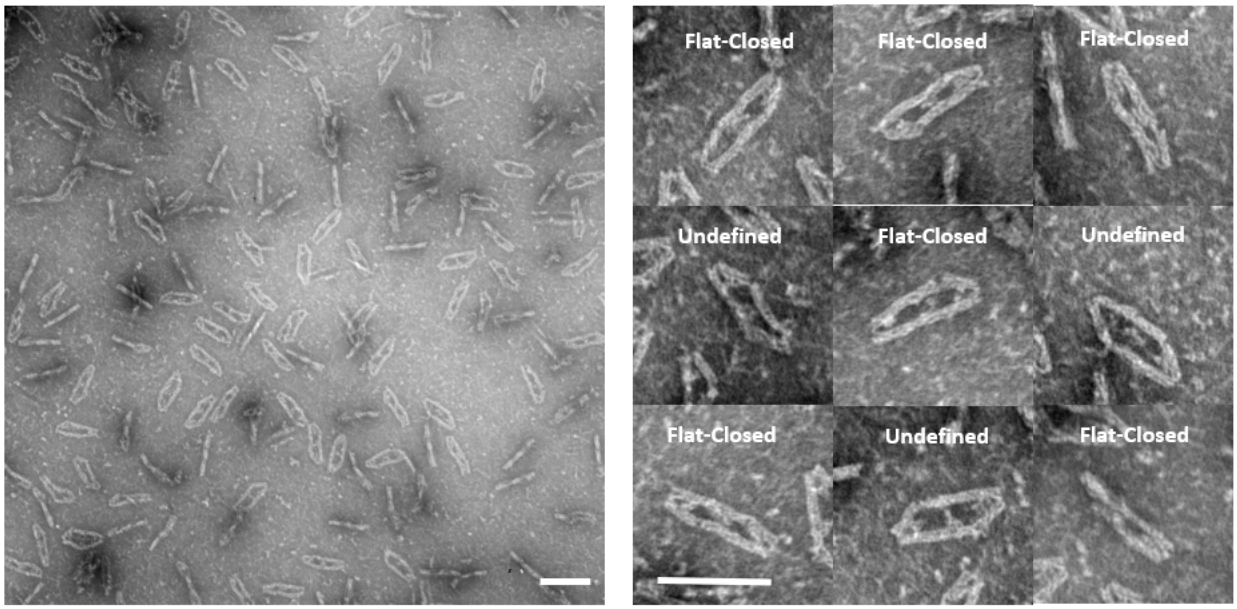
S.11: (Left) Zoom-out TEM image of 1-cycle annealing ramp for preferred shapes upon strut actuation; (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)



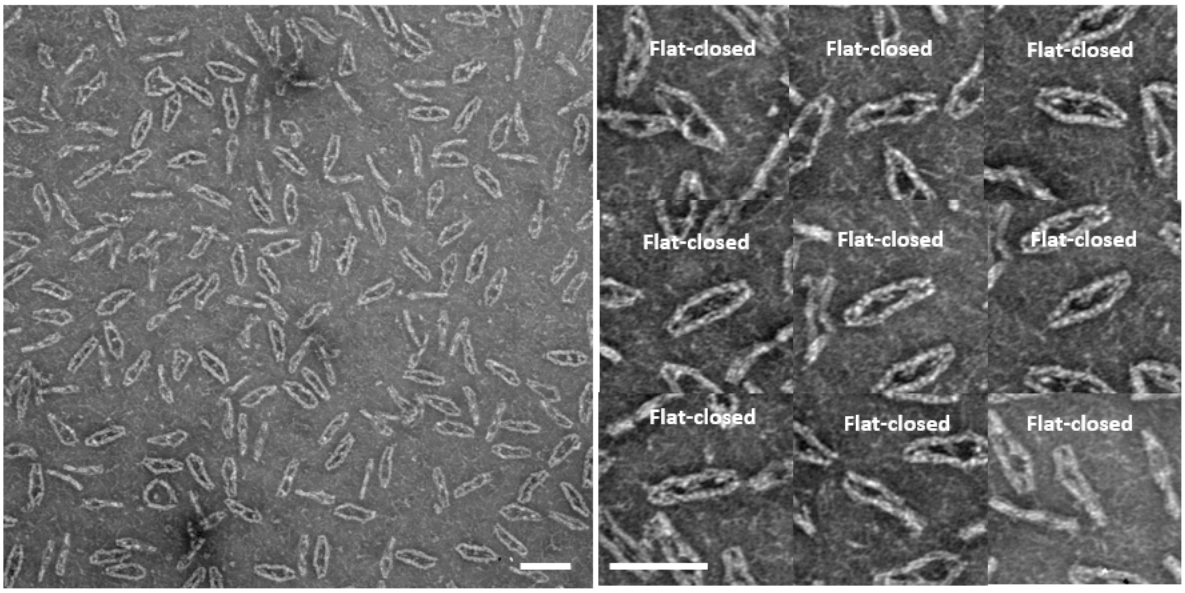
S.12: (Left) Zoom-out TEM image of 2-cycle annealing ramp for preferred shapes upon strut actuation; (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)



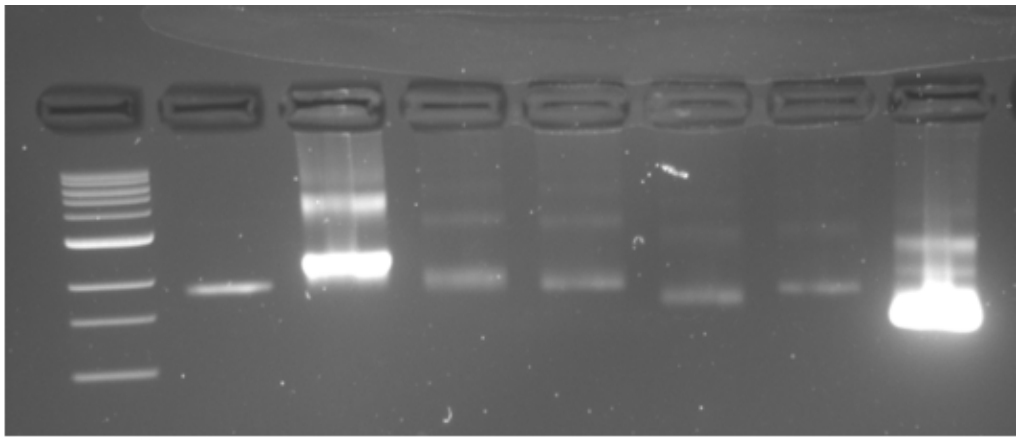
S.13: (Left) Zoom-out TEM image of 3-cycle annealing ramp for preferred shapes upon strut actuation; (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)



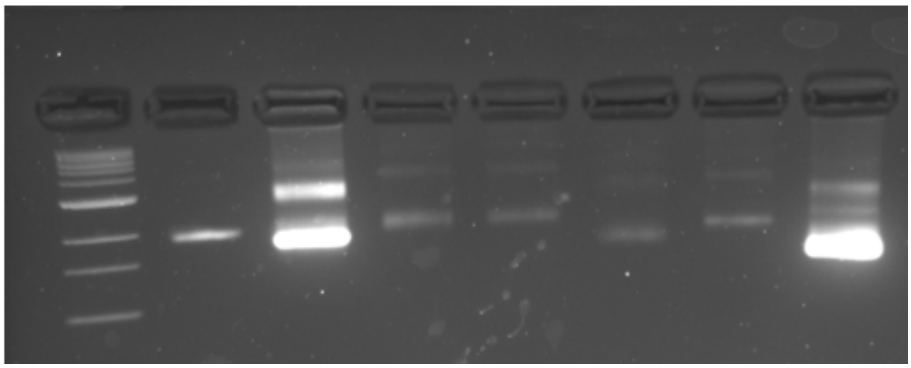
S.14: (Left) Zoom-out TEM image of 2-cycle annealing ramp for replacement from displaced rectangle to flat-closed shape (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)



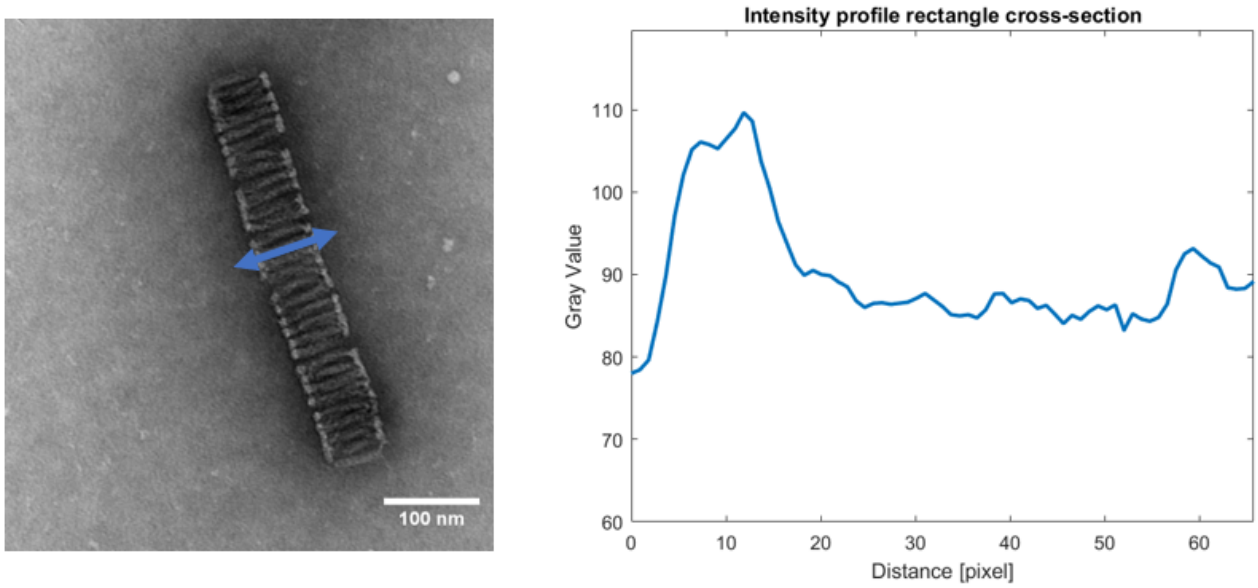
S.15: (Left) Zoom-out TEM image of 2-cycle annealing ramp for replacement from displaced hexagon to flat-closed shape (right) gallery of sorted individual particles from zoom-out TEM image on left (scale bars = 100nm)



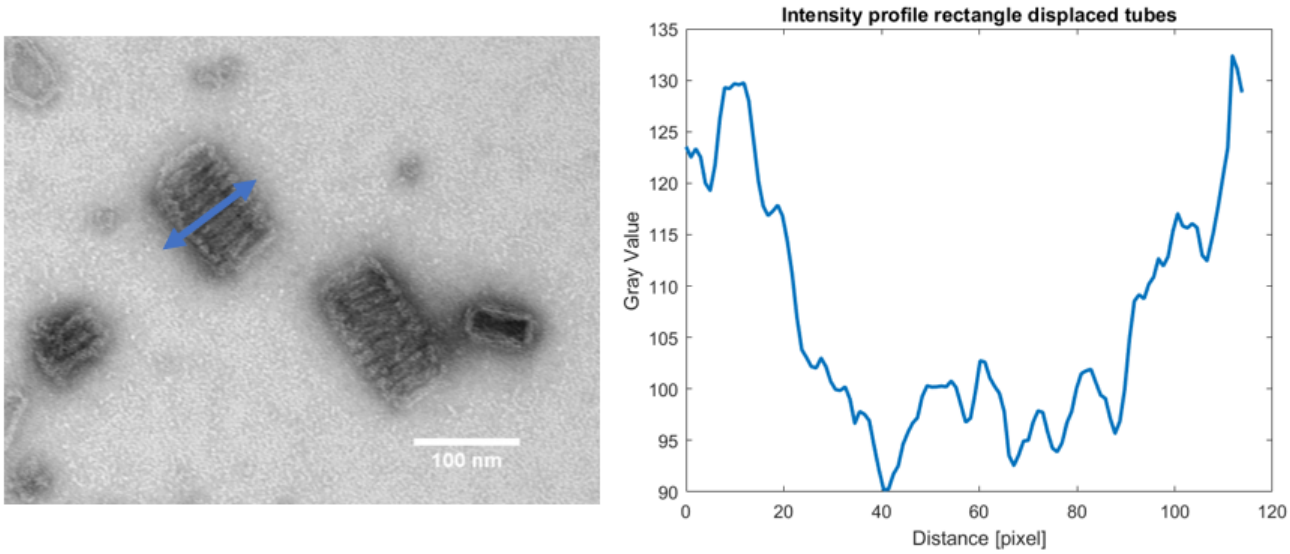
S.16: (left to right) 1kb ladder, 7249 nucleotide scaffold, rectangle fold, rectangle with displacement staples subjected to displacement incubation (RD), rectangle without displacement staples subjected to displacement incubation (RWD), RD with replacement staples subjected to replacement incubation, RWD without replacement staples subjected to replacement incubation, flat-closed fold.



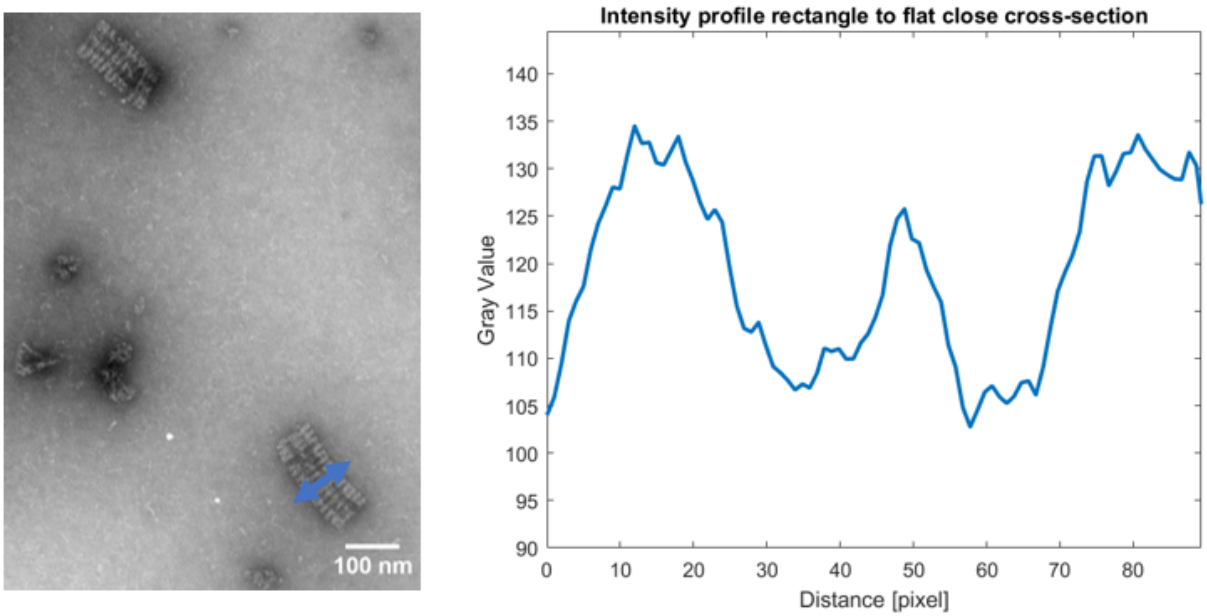
S.17: (left to right) 1kb ladder, 7249 nucleotide scaffold, hexagon fold, hexagon with displacement staples subjected to displacement incubation (HD), hexagon without displacement staples subjected to displacement incubation (HWD), HD with replacement staples subjected to replacement incubation, HWD without replacement staples subjected to replacement incubation, flat-closed fold



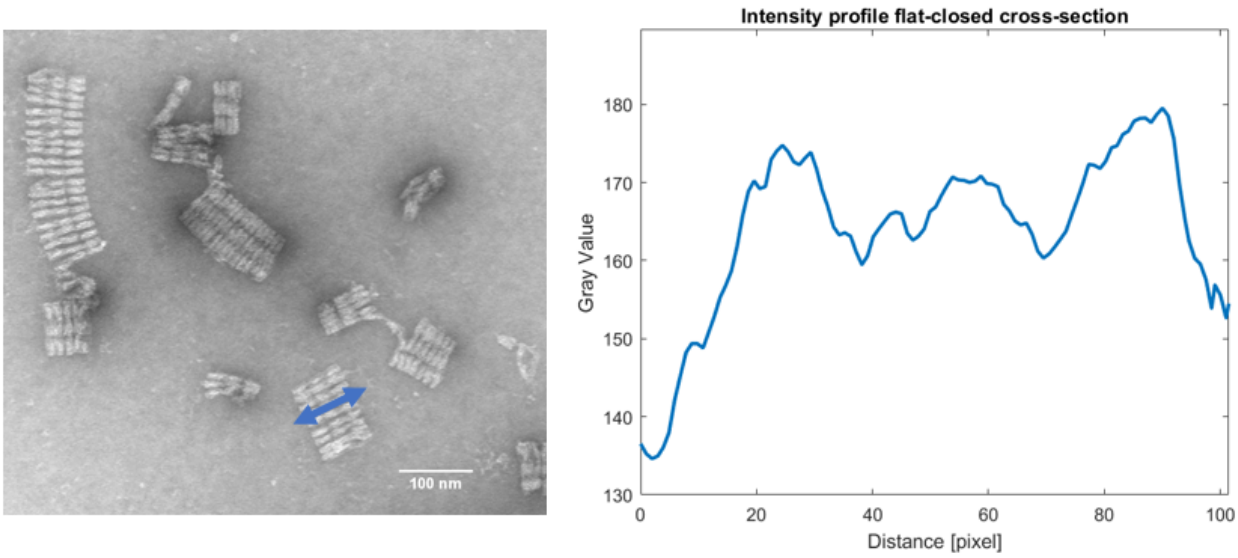
S.18: (left)TEM image of rectangle polymer at 5mM $MgCl_2$ with lateral measurement shown in blue arrow (right) Polymer intensity profile. Scale bar = 100nm



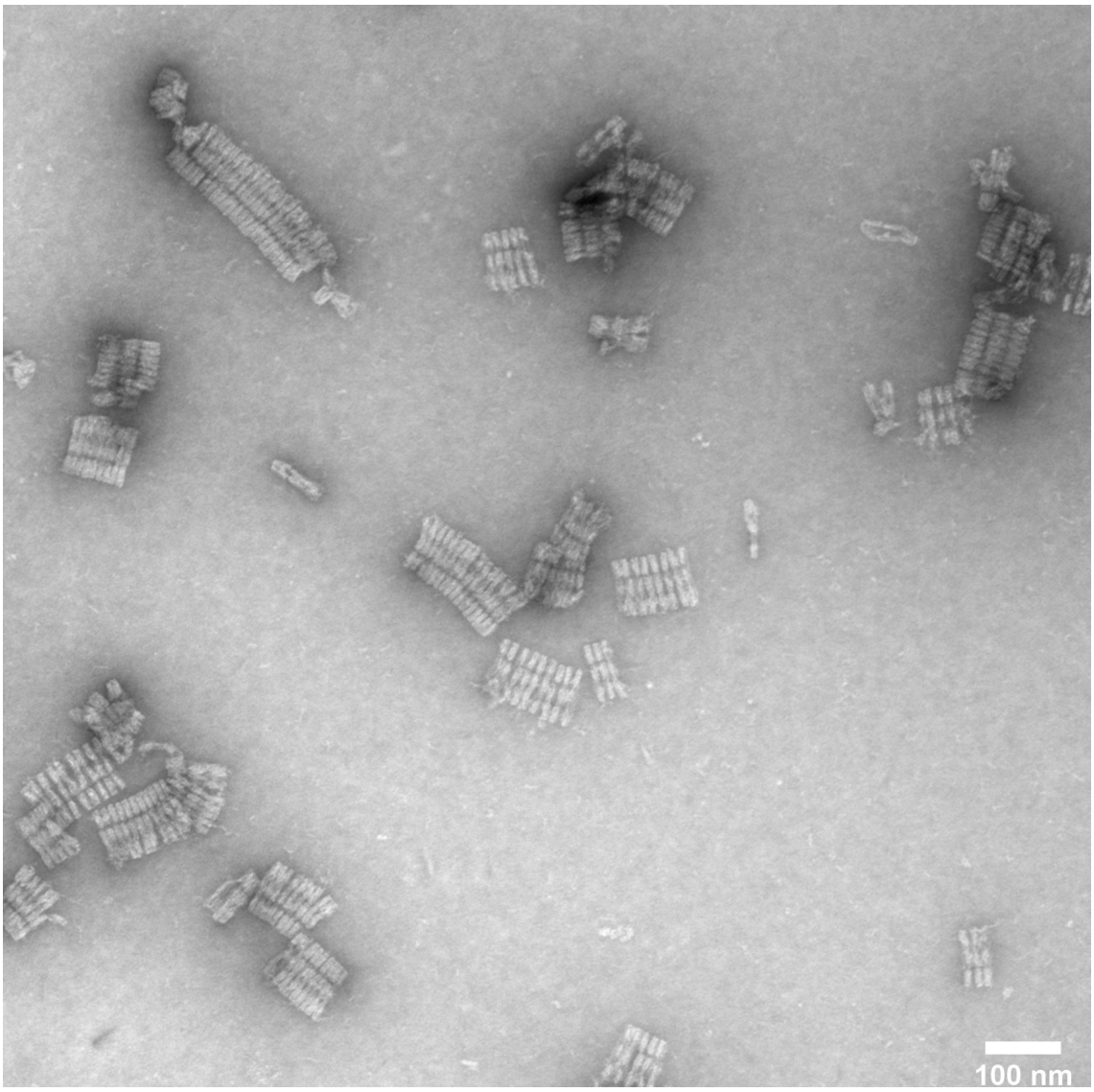
S.19: (left)TEM image of rectangle polymer incubated with displacement strands at 8mM $MgCl_2$ with lateral measurement shown in blue arrow (right) Polymer intensity profile of average of 10 polymers. Scale bar = 100nm



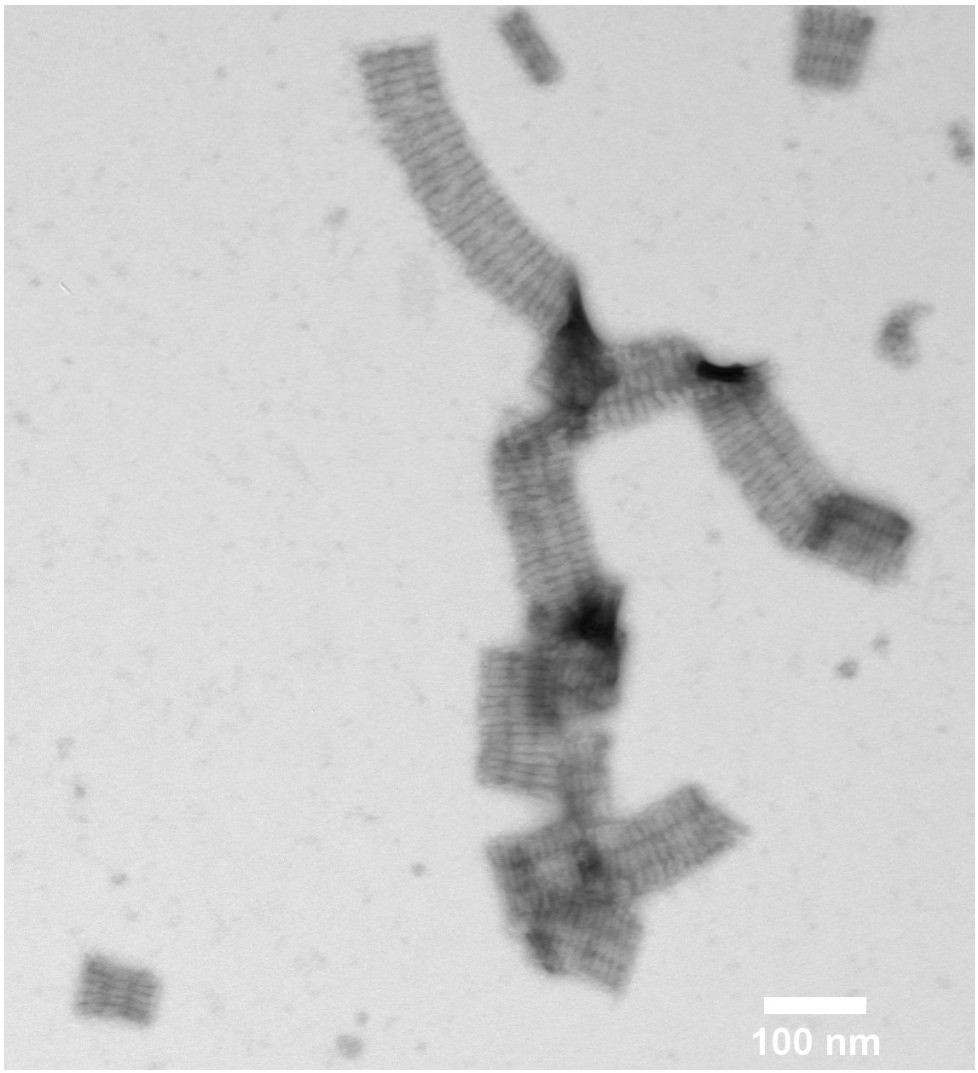
S.20: (left)TEM image of rectangle polymer incubated with displacement strands at 8mM $MgCl_2$ then incubated with transformation staples to flat-closed shape with lateral measurement shown in blue arrow (right) Polymer intensity profile. Scale bar = 100nm



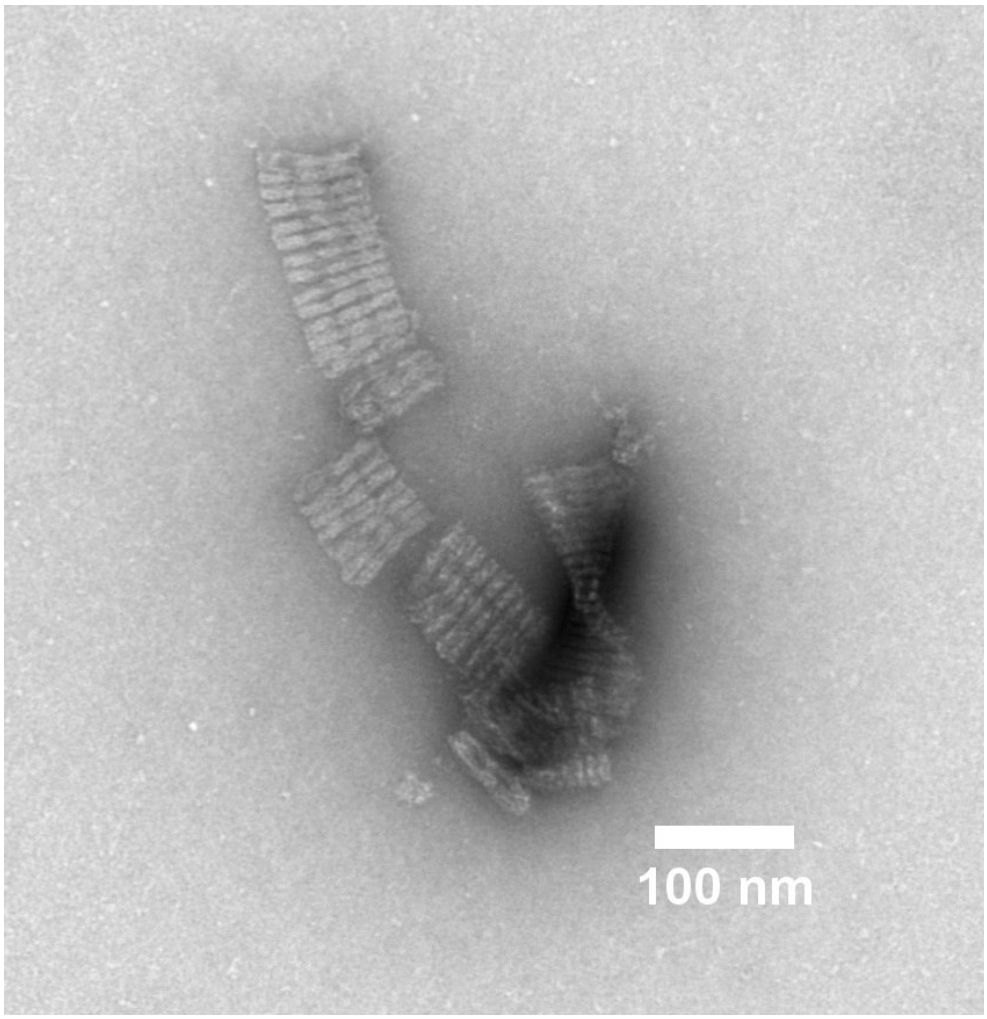
S.21: (left)TEM image of flat-closed polymer at 5mM $MgCl_2$ with lateral measurement shown in blue arrow (right) Polymer intensity profile. Scale bar = 100nm



S.22: TEM image of flat-closed “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 5mM $MgCl_2$. Scale bar = 100nm.

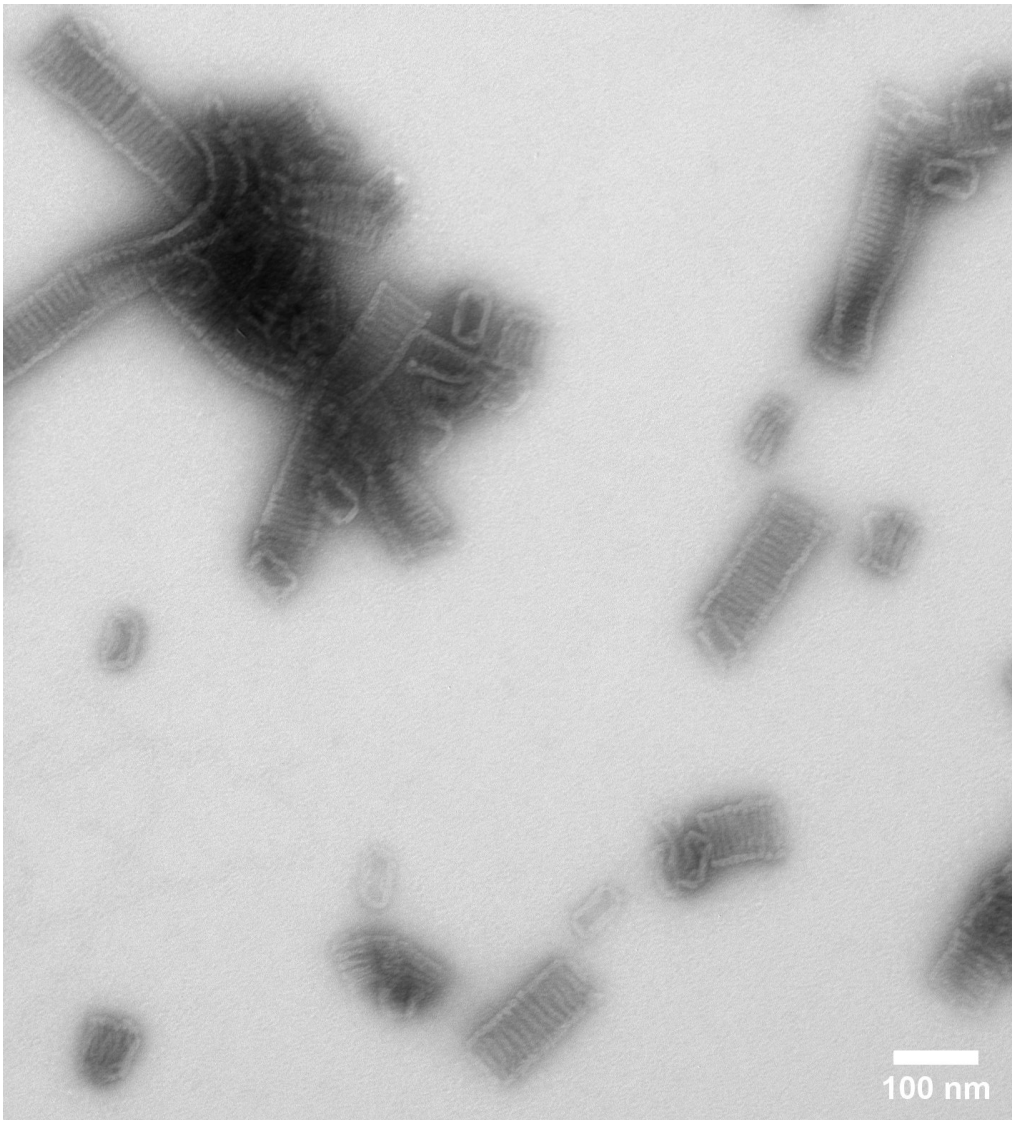


S.23: TEM image of flat-closed “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 10mM $MgCl_2$. Scale bar = 100nm.

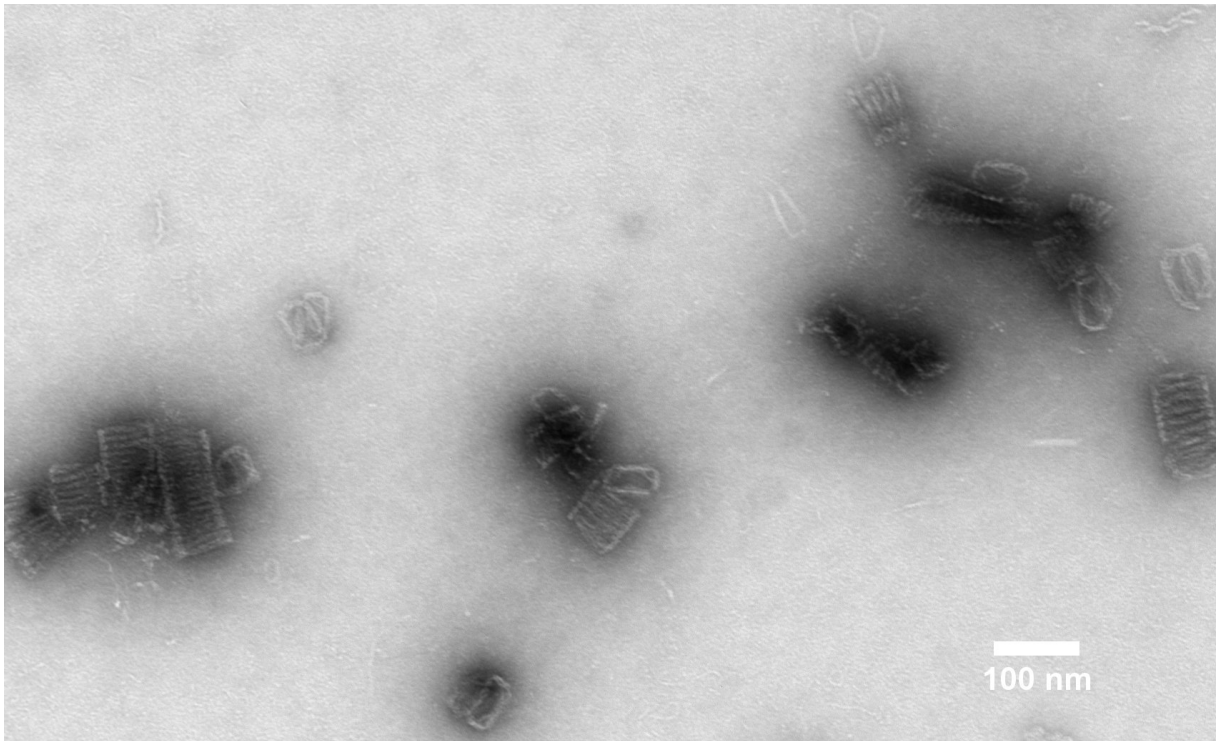


S.24: TEM image of flat-closed “A” and “B” monomers polymerized a 2-cycle annealing incubation with a buffer containing 20mM $MgCl_2$. Scale bar = 100nm.

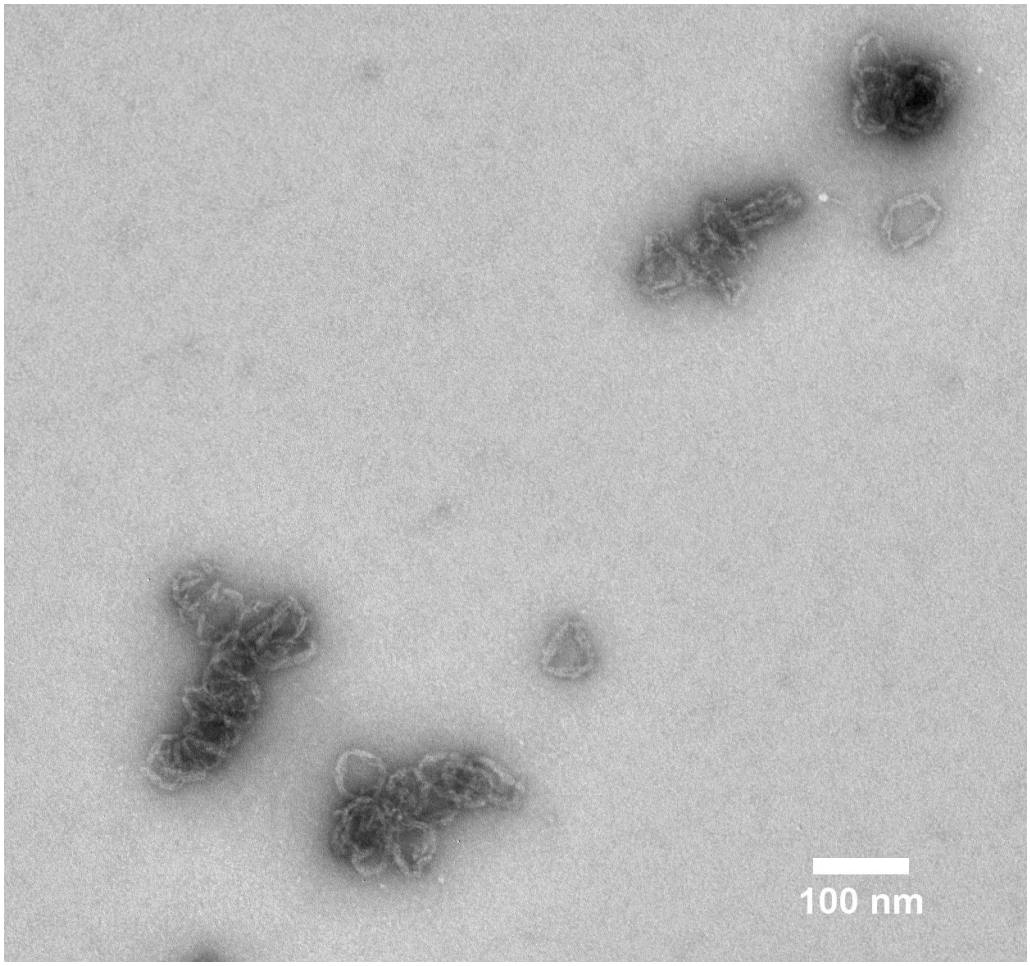
S.25: TEM image of rectangle “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 5mM $MgCl_2$. Scale bar = 100nm.



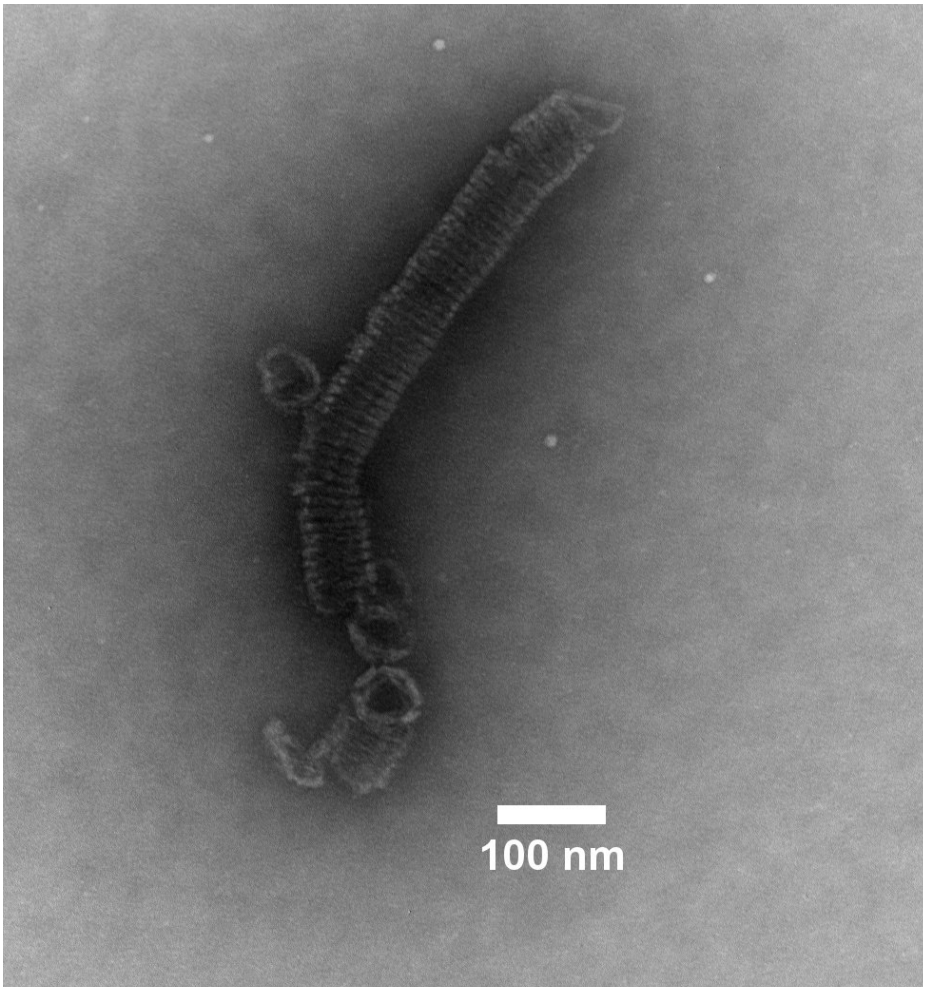
S.26: TEM image of rectangle “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 10mM $MgCl_2$. Scale bar = 100nm.



S.27: TEM image of rectangle “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 20mM $MgCl_2$. Scale bar = 100nm.



S.28: TEM image of hexagon “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 5mM $MgCl_2$. Scale bar = 100nm.



S.29: TEM image of hexagon “A” and “B” monomers polymerized in a 2-cycle annealing incubation with a buffer containing 10 mM $MgCl_2$. Scale bar = 100nm.

Supplementary Information References

1. Douglas SM, Marblestone AH, Teerapittayanon S, Vazquez A, Church GM, Shih WM. Rapid prototyping of 3D DNA-origami shapes with caDNAno. *Nucleic Acids Research*. 2009;37(15):5001-5006. doi:10.1093/nar/gkp436

2. Huang CM, Kucinic A, Johnson JA, Su HJ, Castro CE. Integrated computer-aided engineering and design for DNA assemblies. *Nature Materials*. Published online April 19, 2021:1-8. doi:10.1038/s41563-021-00978-5

3. SantaLucia J. A unified view of polymer, dumbbell, and oligonucleotide DNA nearest-neighbor thermodynamics. *Proceedings of the National Academy of Sciences*. 1998;95(4):1460-1465. doi:10.1073/pnas.95.4.1460

4. SantaLucia John, Allawi HT, Seneviratne PA. Improved Nearest-Neighbor Parameters for Predicting DNA Duplex Stability. *Biochemistry*. 1996;35(11):3555-3562. doi:10.1021/bi951907q

5. Banerjee D, Tateishi-Karimata H, Ohyama T, et al. Improved nearest-neighbor parameters for the stability of RNA/DNA hybrids under a physiological condition. *Nucleic Acids Research*. 2020;48(21):12042-12054. doi:10.1093/nar/gkaa572

6. Sugimoto N, Nakano S ichi, Katoh M, et al. Thermodynamic Parameters To Predict Stability of RNA/DNA Hybrid Duplexes. *Biochemistry*. 1995;34(35):11211-11216. doi:10.1021/bi00035a029

7. Nearest Neighbor Calculator for Nucleic Acids. Accessed November 23, 2022. http://www.konan-fiber.jp/hp/sugimoto/contents/NN/NearestNeighborCalculator.htm