Supplementary Information

for

Stacking of Short DNA Induces the Gyroid Cubic-to-Inverted Hexagonal Phase Transition in Lipid–DNA Complexes

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Figure S1. Synchrotron small-angle X-ray scattering scan taken at 51.4 °C for isoelectric complexes of 5 bp DNAs with dAdT overhangs (black line). The data show coexistence of the gyroid cubic ($Q_{II}^{G,\ sDNA}$) and the inverted hexagonal (H_{II}^{C}) phase. The first peaks of the $Q_{II}^{G,\ sDNA}$ and the H_{II}^{C} phases (centered at q_{211} and q_{10}, respectively) were fit to a double Lorentzian line shape (orange line). The areas of the peaks were integrated between the limits indicated by the arrowheads and the percentage of cubic phase ($\%Q_{II}^{G,\ sDNA}$) was calculated as $\%Q_{II}^{G,\ sDNA} = A^{Q}(q_{211})/[A^{Q}(q_{211}) + A^{H}(q_{10})]$, where $A^{Q}(q_{211})$ and $A^{H}(q_{10})$ are the areas under the peaks centered at q_{211} and q_{10}, respectively.

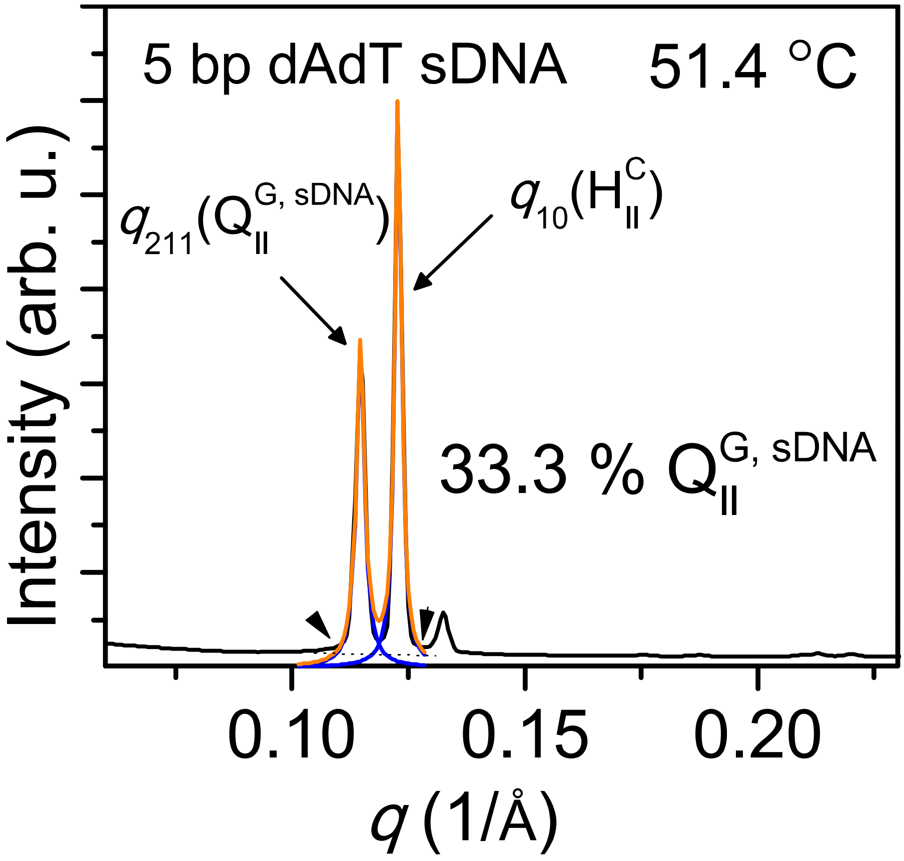


Table S1. Sequences of the sense (s) and antisense (as) strands of the sDNA molecules used in this study.

Sequence		**Duplex name**
s	ACGCTAT	5bp dAdT
as	AGCGTAT	
s	ACGCT	5bp blunt
as	AGCGT	
s	ACGCTTT	5bp dTdT
as	AGCGTTT	
s	CTTACGCTGAGAT	11bp dAdT
as	CTCAGCGTAAGAT	
s	CTTACGCTGAG	11bp blunt
as	CTCAGCGTAAG	
s	CTTACGCTGAGTT	11 bp dTdT
as	CTCAGCGTAAGTT	
s	ATCACTTACGCTGAGTACTTCGAAAT	24bp dAdT
as	TTCGAAGTACTCAGCGTAAGTGATAT	
s	ATCACTTACGCTGAGTACTTCGAA	24bp blunt
as	TTCGAAGTACTCAGCGTAAGTGAT	
s	ATCACTTACGCTGAGTACTTCGAATT	24bp dTdT
as	TTCGAAGTACTCAGCGTAAGTGATTT	
s	ACAGATGCACATATCGAGGTGGACATCACTTACGCTGAGTACTTCGAAAT	48bp dAdT
as	TTCGAAGTACTCAGCGTAAGTGATGTCCACCTCGATATGTGCATCTGTAT	
s	ACAGATGCACATATCGAGGTGGACATCACTTACGCTGAGTACTTCGAA	48bp blunt
as	TTCGAAGTACTCAGCGTAAGTGATGTCCACCTCGATATGTGCATCTGT	
s	ACAGATGCACATATCGAGGTGGACATCACTTACGCTGAGTACTTCGAATT	48bp dTdT
as	TTCGAAGTACTCAGCGTAAGTGATGTCCACCTCGATATGTGCATCTGTTT	

Calculation of the concentration of sDNA strands in the CL–sDNA complex pellets

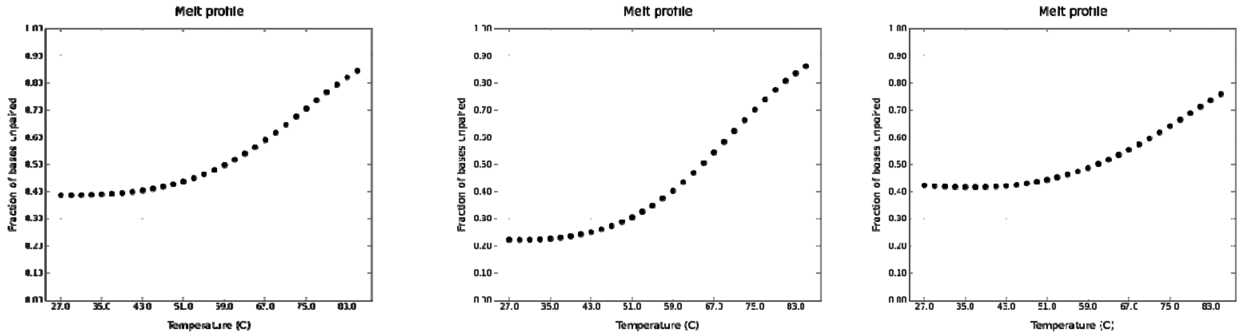
The volume of the CL–sDNA sample (V_p) was calculated by approximating the pellet as a sphere of 1 mm diameter, yielding $V_p = 0.52$ µL. The molar mass of the sDNA strands (M_{sDNA}) was approximated by multiplying the number of bases with the average molar mass of a base of 330 g/mol. Each sample contained 50 µg of sDNA (m_{sDNA}), corresponding to an amount of sDNA (in mol) of $n_{sDNA} = m_{sDNA}/M_{sDNA}$. The concentration of each sDNA strand in the sample pellet, C_{sDNA}, then is $C_{sDNA} = 0.5 \times n_{sDNA}/V_p$.

As an example, a sample containing blunt 5 bp sDNA with M_{sDNA}=5×330=1650 g/mol will have n_{sDNA} = 50 µg/(1650 g/mol) = 30.3 nmol and C_{sDNA} = 0.5 × 30.3 nmol / (0.52 µL) = 28.9 mM.

Figure S2. Melting profiles (percentage of unpaired strands vs. Temperature) for all sDNA used in this work estimated using the *Nupack* software package (J. N. Zadeh et al. *J. Comput. Chem.*, 2011, 32, 170–173).

5 bp (1 M NaCl)

dAdT (20.6 mM) Blunt (28.9 mM) dTdT (20.6 mM)



11 bp (1 M NaCl)

dAdT (11.1 mM) Blunt (13.2 mM) dTdT (11. 1 mM)

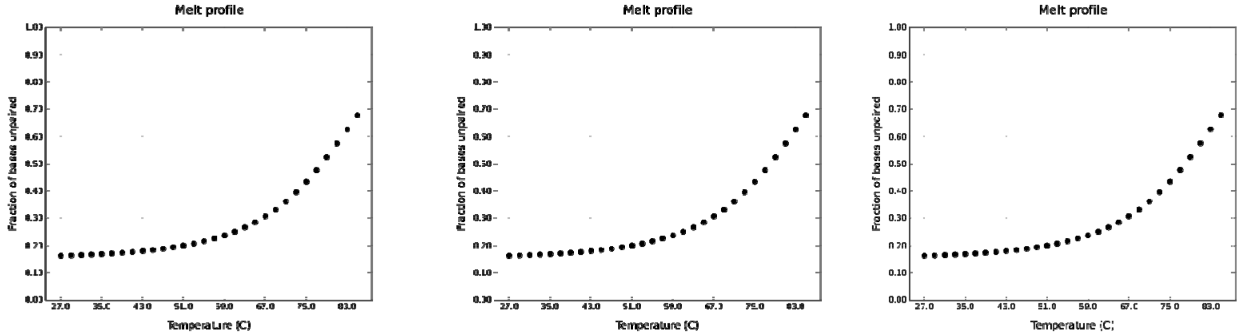
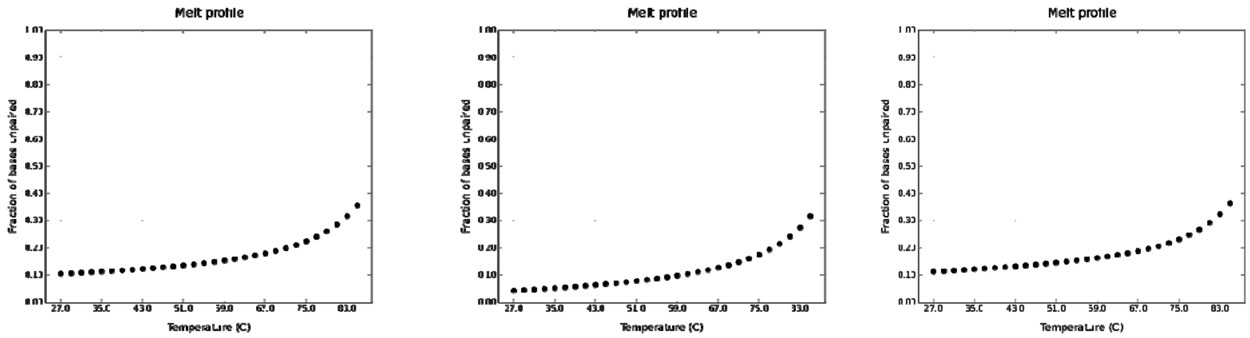


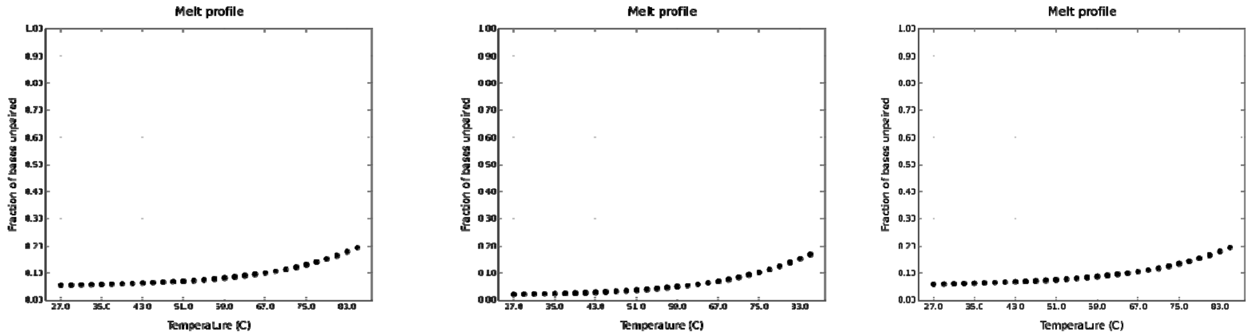
Figure S2 ctd.

24 bp (1 M NaCl)



dAdT (5.6 mM) Blunt (6.0 mM) dTdT (5.6 mM)

48 bp (1 M NaCl)



dAdT (2.9 mM) Blunt (3.0 mM) dTdT (2.9 mM)

Table S2. sDNA dehybridization temperatures (T_m, the temperature where 50% of the bases are unpaired) for all sDNAs determined from calculated melting profiles (Figure S2).

sDNA	T_m (°C)
5 bp dAdT	59.0
5 bp blunt	64.5
5 bp dTdT	61.0
11 bp dAdT	78.0
11 bp blunt	76.5
11 bp dTdT	77.5
24 bp dAdT	> 85
24 bp blunt	> 85
24 bp dTdT	> 85
48 bp dAdT	> 85
48 bp blunt	> 85
48 bp dTdT	> 85