Supporting Information

Self-Assembly of DNA G-Quadruplex Nanowires: A Study of Mechanism towards Micro-meter Length

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Table S1. The composition of the buffer solution

NO.	Li^+ (mM)	K^+ (mM)	Sr^{2+} (mM)	Mg^{2+} (mM)
1	50	50	10	/
2	10	10	/	/
3	100	10	/	/
4	50	50	/	/
5	10	100	/	/
6	50	50	/	10
7	10	50	50	/

Table S2. DNA sequences of modified dG4

DNA	Sequences (5’ to 3’)
5’P-G4	p-GGGG*
G4-3’P	GGGG-p
G4T	GGGGT
TG4	TGGGG
TG4T	TGGGGT

* low case “p” mean phosphorylation at 5’- or 3’-end.

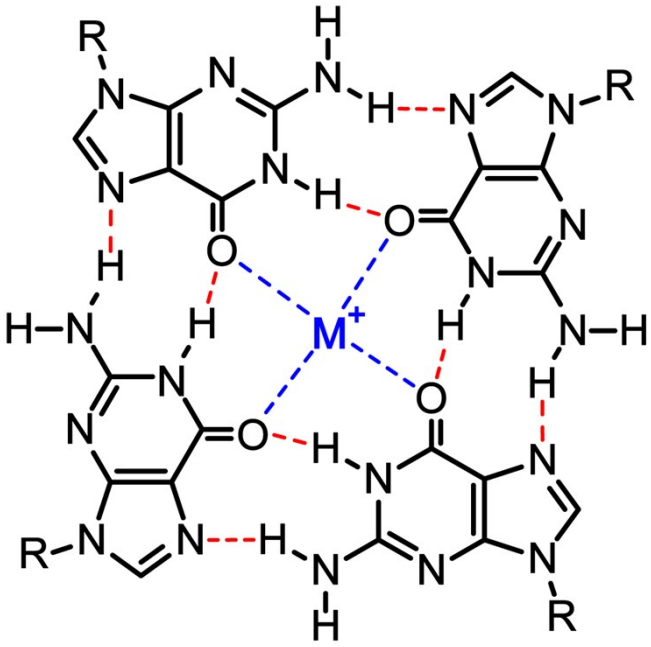


Figure S1. The chemical structure of a G-tetrad

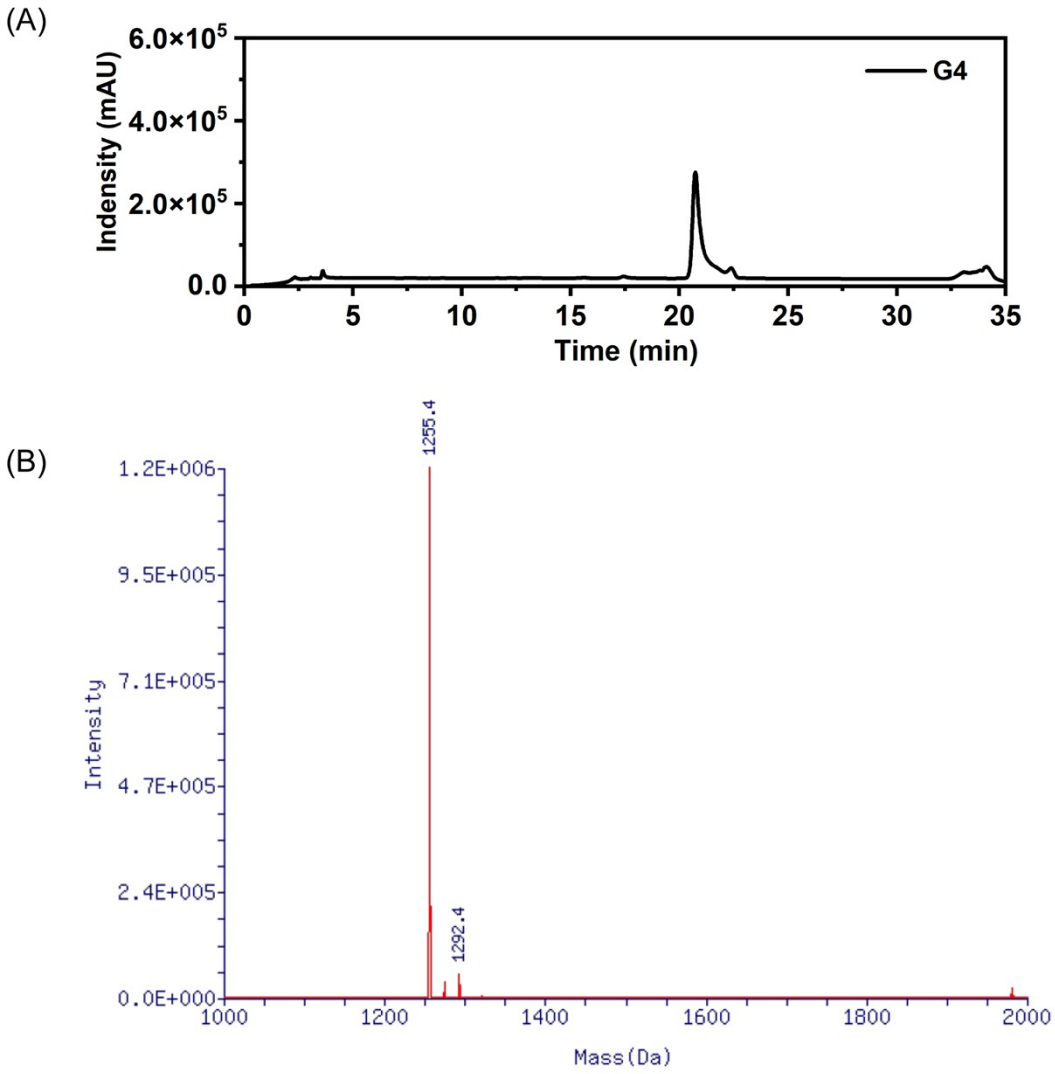


Figure S2. Characterization of the dG4 (5'-GGGG-3'). HPLC traces (A) and ESI-Mass spectrum (B).

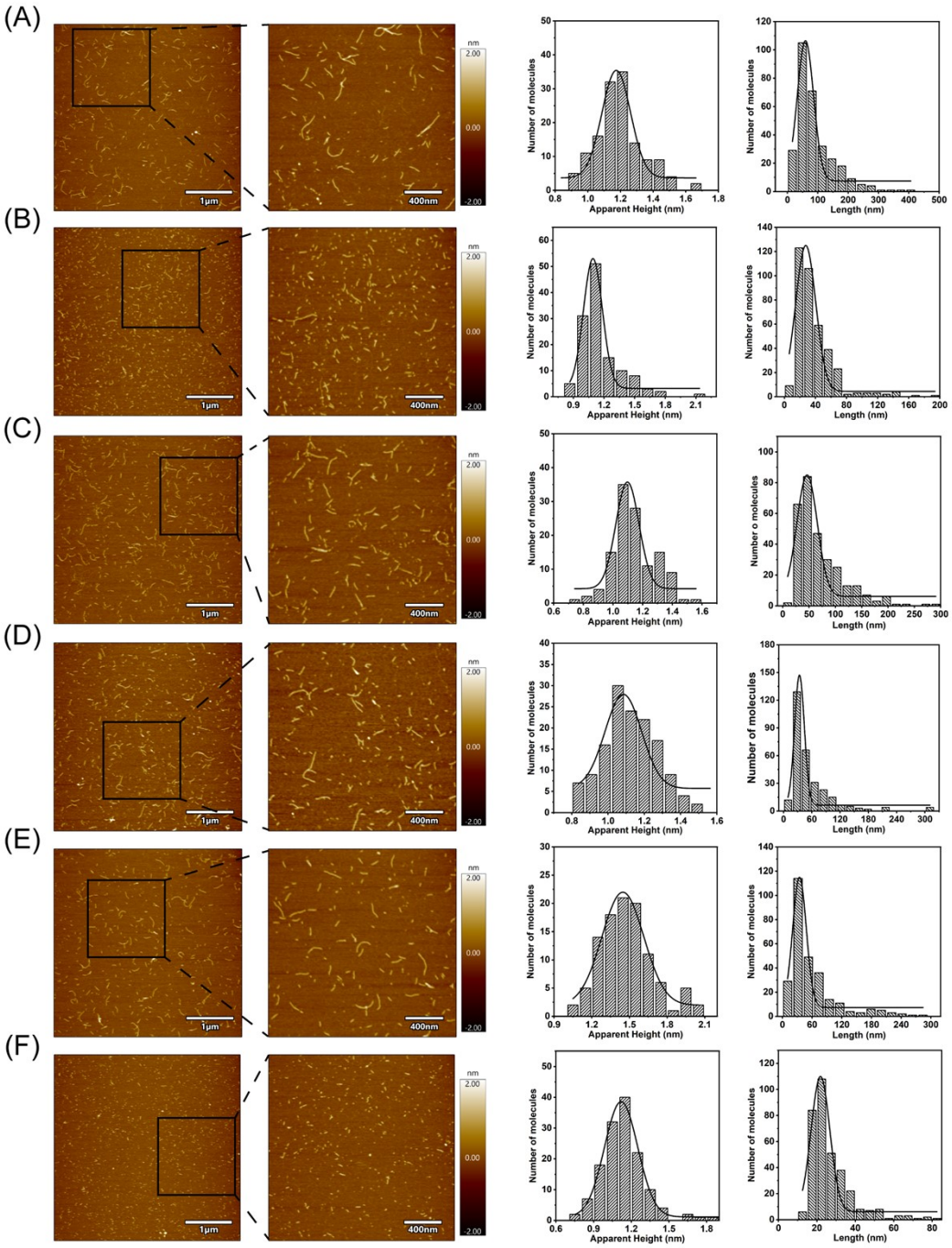


Figure S3. AFM images and statistical analyses for heights and lengths of corresponding G-wires grown in different protocol solutions. Measured G-wires are wG-2 (A), wG-3 (B), wG-4 (C), wG-5 (D), wG-6 (E), wG-7 (F).

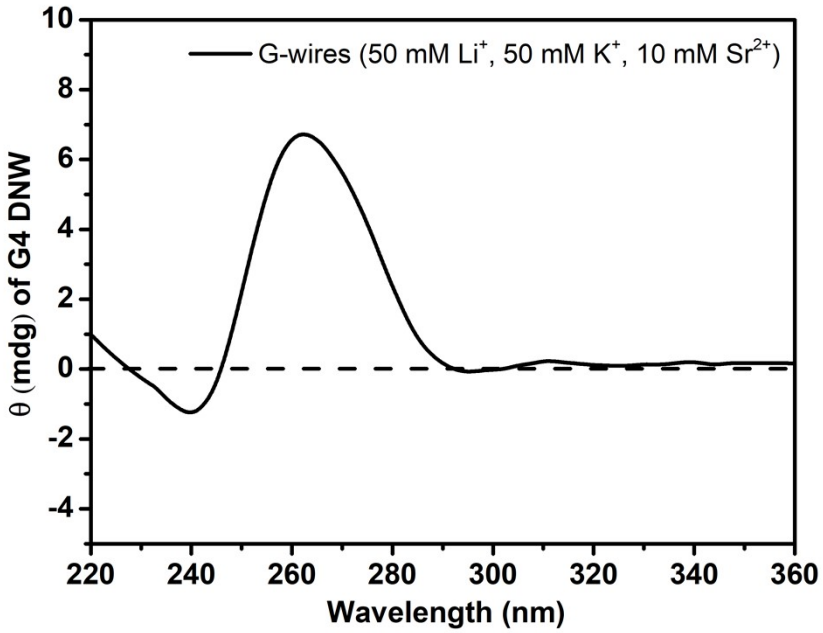
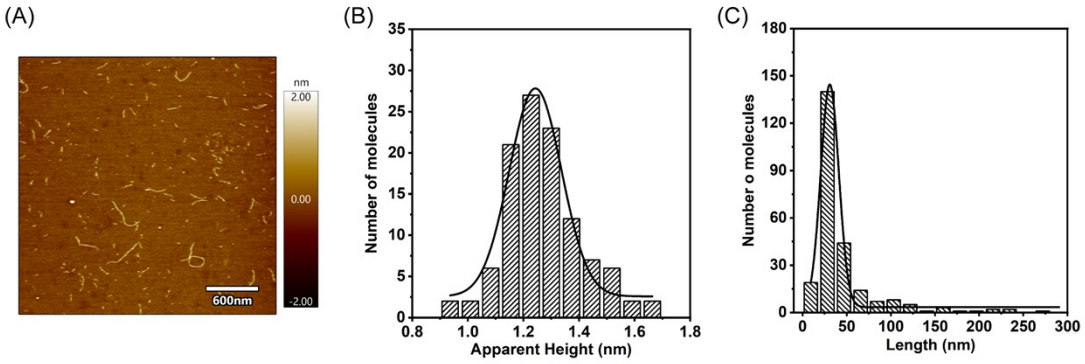


Figure S4. CD spectrum of G-wires in 50 mM Li^{+}, 50 mM K^{+}, 10 mM Sr^{2+}.



(D)

	Growth temperature	
	4 °C	25 °C
Average height (nm)	1.1	1.3
Average length (nm)	127	31

Figure S5. G-wires formation challenged by incubating temperature. AFM image (A) of G-wires incubated at 25 °C. Height (B) and length (C) histograms of G-wire in (A). Height and length comparison (D) of G-wires incubated at 4 °C and 25 °C.

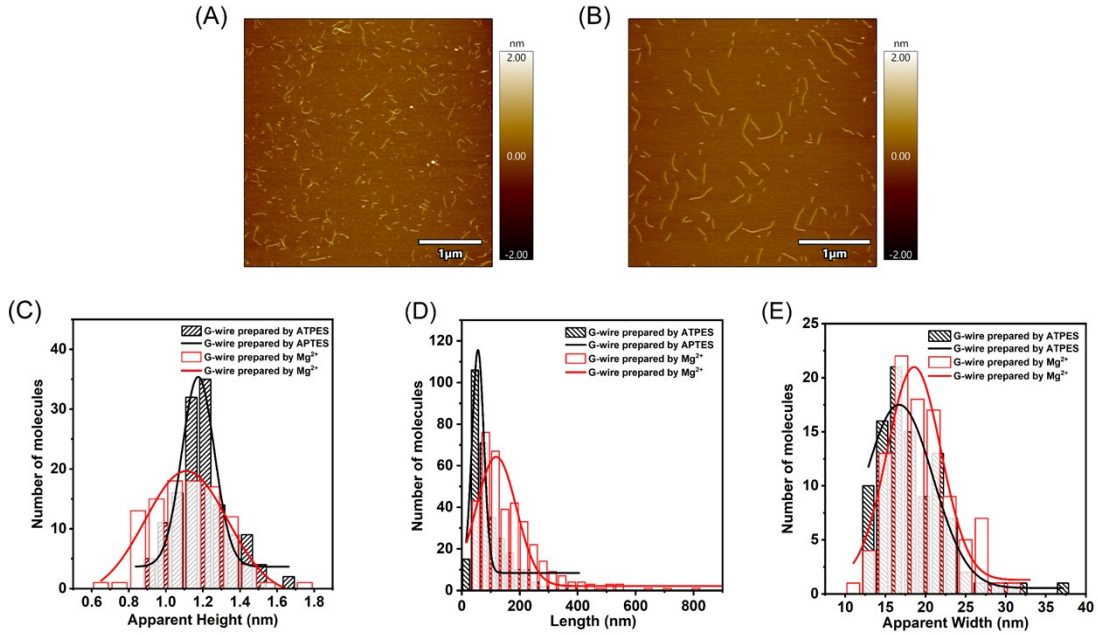


Figure S6. Longer G-wires formed on the mica surface. AFM images of G-wires deposited onto mica surface via APTES binding (A) and via Mg^{2+} treatment (B). Height (C), length (D) and width (E) histograms of G-wires in (A) and (B). Measured G-wire formed in 50 mM Li^{+}, 50 mM K^{+}, 10 mM Mg^{2+}.

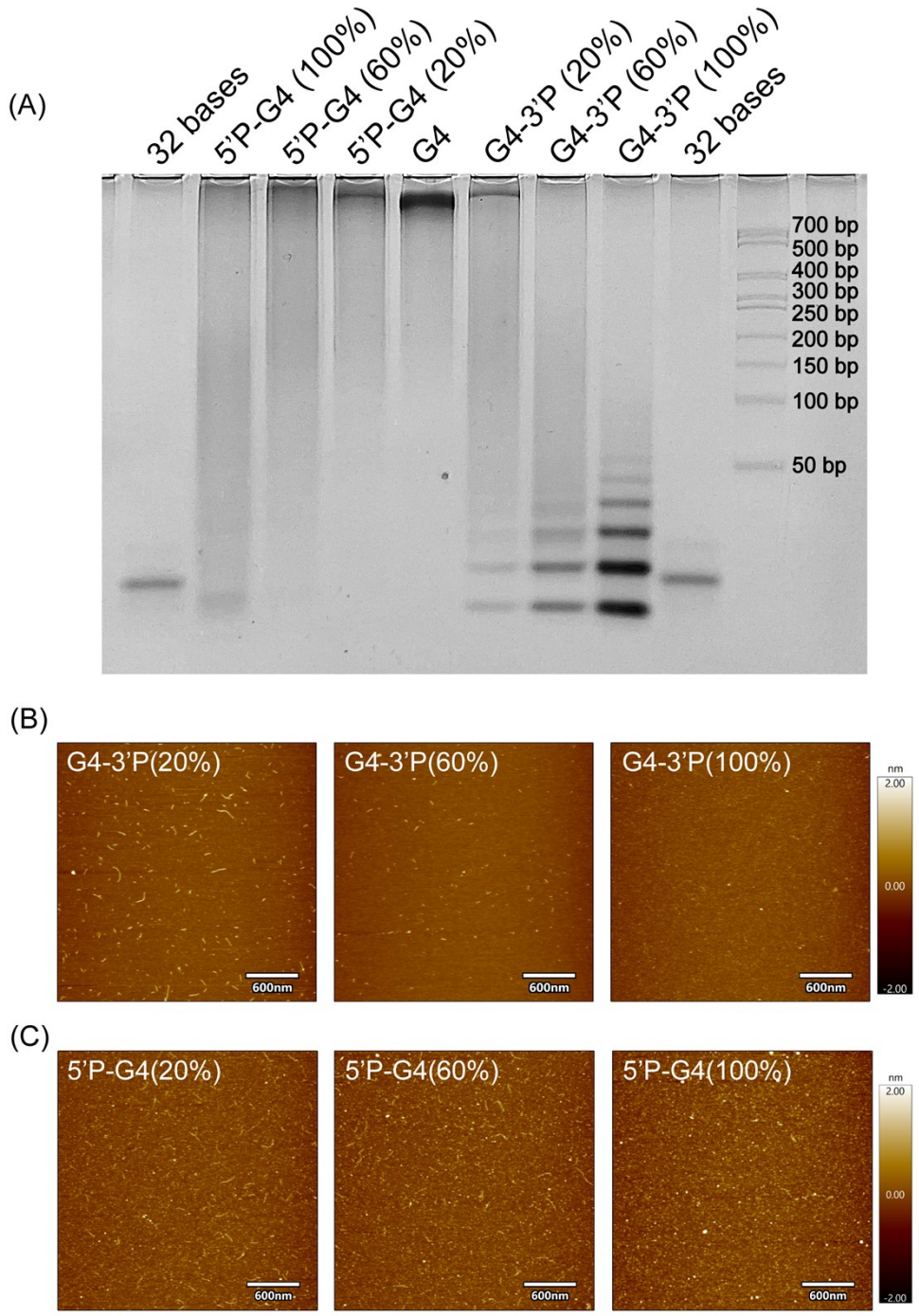


Figure S7. Characterization of G-wire modified by phosphate groups on dG4's end. Native PAGE analysis (A) and AFM images of G-wires self-assembled from a mixture of dG4 and 3' (B) or 5' (C) terminal phosphate groups modified dG4 at radio of 20%, 60% and from phosphate groups modified dG4 only.

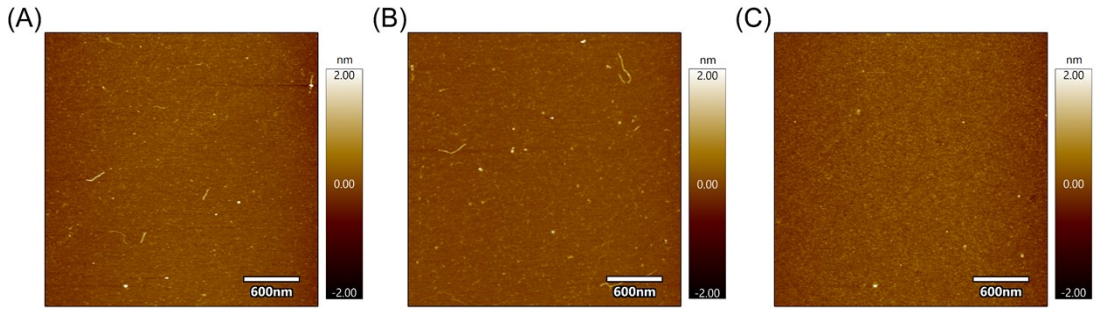


Figure S8. AFM images of G-wires formed by annealing dTG4 (A), dG4T (B) and dTG4T (C).

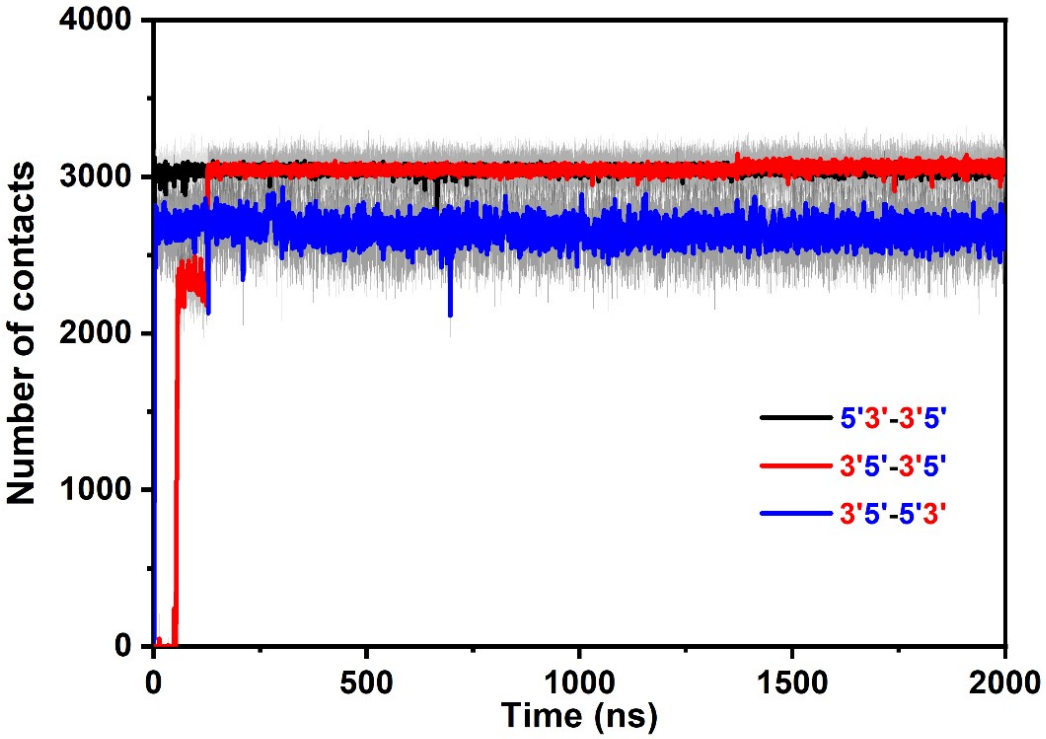


Figure S9. Number of contacts between dimers as a function of simulation time. The running smooth of the contacts are plotted in black, red, and blue, respectively.

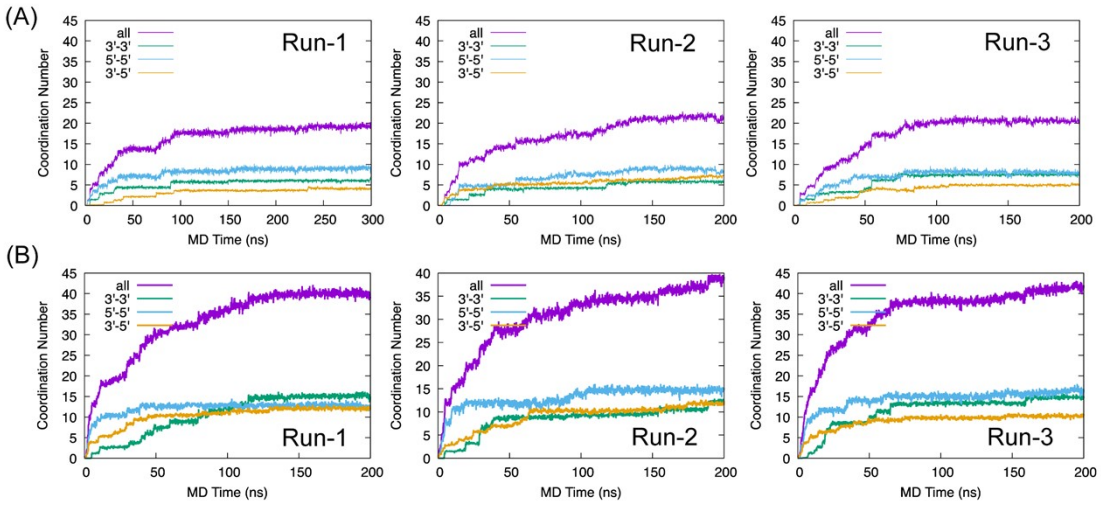


Figure S10. The coordination number for three different stacking modes (3'-3', 5'-5', and 3'-5') and cumulative coordination number as a function of simulation time within the KCl (A) or KCl/Sr_2Cl (B) conditions.

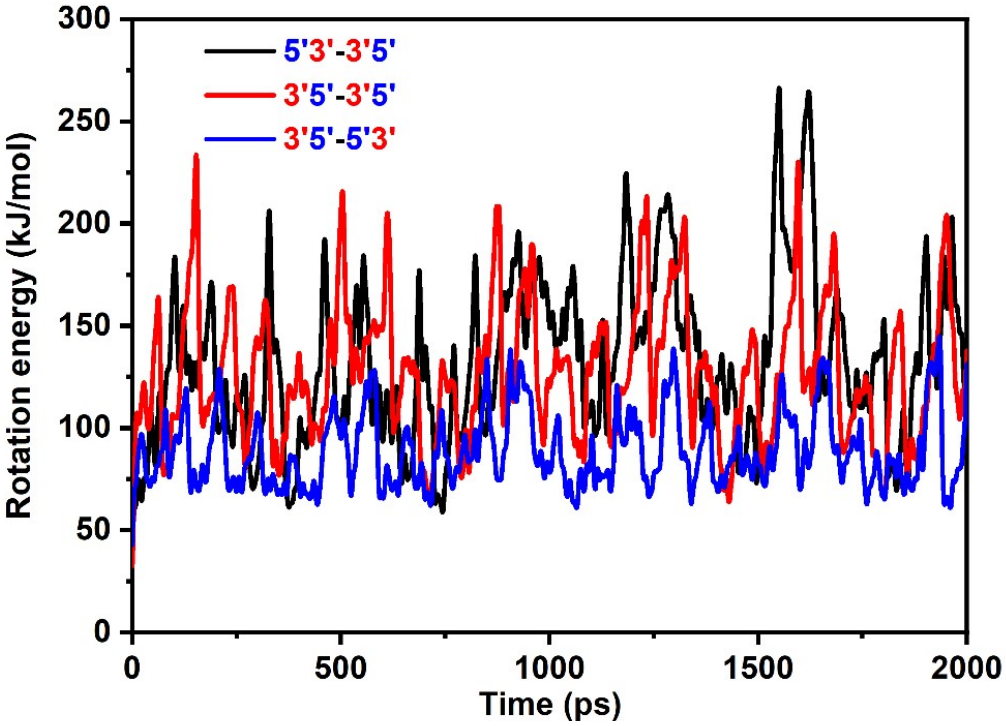


Figure S11. The rotational energy between two monomers within a G4 dimer as a function of simulation time.

Supplementary video (still image):