Supplementary Material (ESI) for Chemical Communications

Electronic Supporting Information:

Charge Transfer in DNA Assembly: Effects of Sticky End

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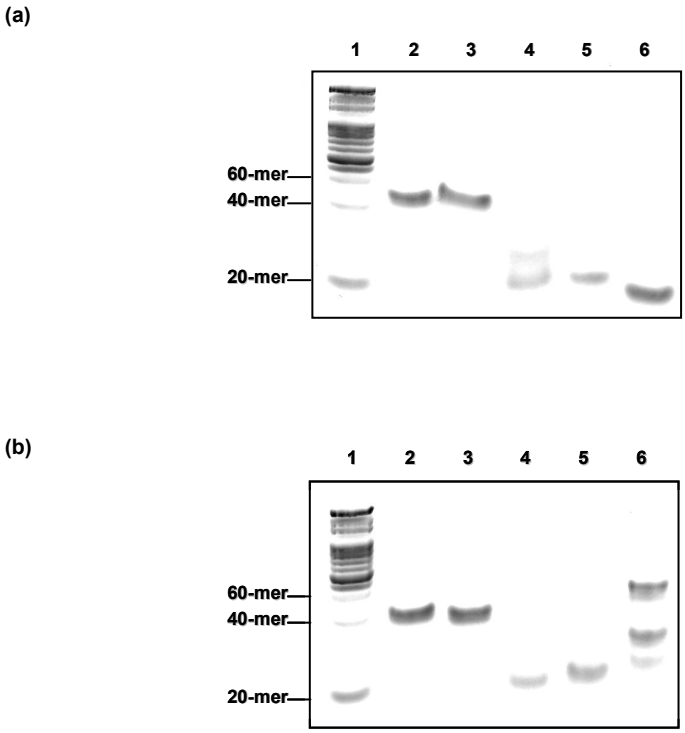

Figure S1. Characterization of the DNA assemblies. 15% Nondenaturing PAGE analysis. (a) Lane 1: 20-bp DNA ladder; lane 2: **ST10**; lane 3: **ST8**; lane 4: **ST6**; lane 5: **ST4**; lane 6: **ST2**. (b) Lane 1: 20-bp DNA ladder; lane 2: **N1 + P1** (**ST10**); lane 3: **N2 + P2**; lane 4: **N1+P2**; lane 5: **N2+P1**; lane 6: **N1+ C +P2**.

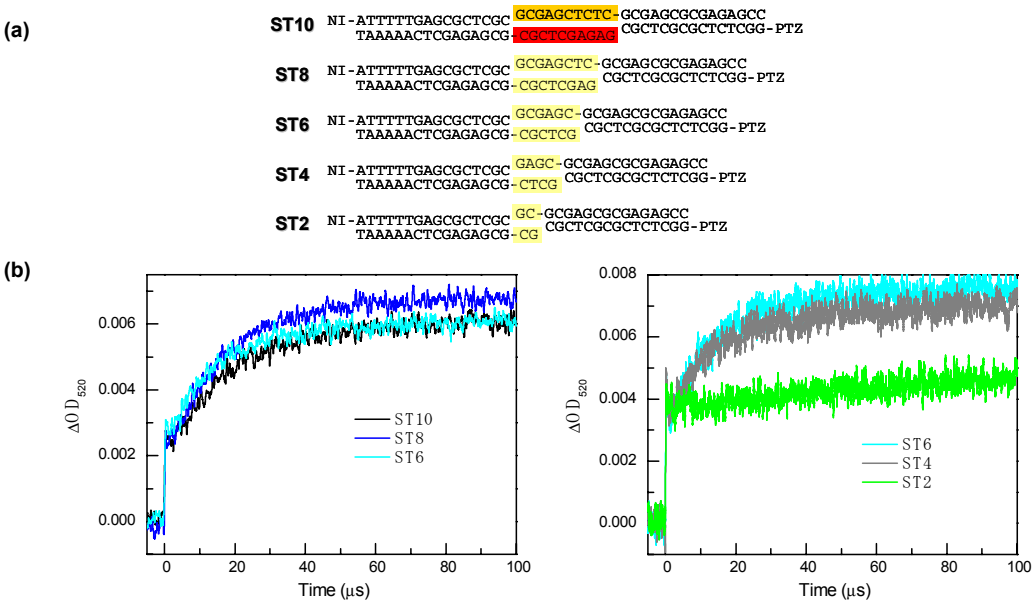

Figure S2. (a) Schematic illustration of DNA assembly for the examination of the effects of sticky end length: **ST10**, **ST8**, **ST6**, **ST4** and **ST2**. (b) Time profiles of the transient absorption of $\mathbf{PTZ}^{\bullet+}$ monitored at 520 nm during the 355 nm laser flash photolysis of **ST10** (black), **ST8** (blue), **ST6** (cyan), **ST4** (gray) and **ST2** (gray), respectively. The represented profiles were obtained from the accumulation of 32 laser shots.

Experimental

DNA Synthesis.

All reagents for DNA synthesis were purchased from Glen Research. Cyanoethyl phosphoramidites of *N*-(3-hydroxy-propyl)-1,8-naphthalimide and 10-(2-Hydroxyethyl)phenothiazine were synthesized as previously reported[1,2] DNA used in this study was synthesized on an Applied Biosystems DNA synthesizer with standard solid-phase techniques and purified on a JASCO HPLC with a reverse-phase C-18 column with an acetonitrile/50 mM ammonium formate gradient. Duplex solutions were prepared by mixing equimolar amounts of the desired DNA complements and gradually annealing with cooling from 80°C to room temperature. Cooling was performed over 16 h. DNAs conjugated with NI and PTZ at the 5' end were synthesized according to a previous procedure. 5’ end phosphorylated oligonucleotides were synthesized by Chemical Phosphorylation Reagents Ⅱ (Glen Research). DNA ligation reaction was carried out as previously described.[3] In briefly, a sample solution (25 μL) containing 2 μM NI- and PTZ-modified DNAs, 2μM phosphorylated DNA strands (sample, P), 66 mM Tris-HCl buffer (pH 7.6), 6.6 mM $MgCl_2$, 0.1 M NaCl, 10 mM DTT, and 1 mM ATP was heated at 80 °C for 10 min, then gradually cooled down to 16 °C (1.0 °C/min) by a thermal cycler (BIORAD). T4 DNA ligase (20 unit, TOYOBO)

was added to the mixtures, and the reaction was carried out at 16 °C for 16 h. After the reaction, the mixture was heated at 85 °C and desalted with Micro Bio-Spin Chromatography Column (BIORAD) before sample preparation for laser flash photolysis.

Laser Flash Photolysis Experiments.

Nanosecond transient absorption measurements were performed as previously described.[4-7] The third-harmonic oscillation (355 nm, fwhm of 4 ns, 20 mJ/pulse) from a Q-switched Nd:YAG laser (Continuum, Surelight) was used for the excitation light. A xenon flash lamp (Osram, XBO-450) was focused into the sample solution as the probe light for the transient absorption measurement. Time profiles of the transient absorption in the UV-visible region were measured with a monochromator (Nikon, G250) equipped with a photomultiplier (Hamamatsu Photonics, R928) and digital oscilloscope (Tektronics, TDS-580D).

Gel shift assay.

50 μM each of DNA strands were annealed in 100 mM NaCl, 20 mM Na phosphate buffer (pH 7.0) from 95 °C to room temperature. After incubation, an amount of glycerol (50%) equal to 10% of the reaction volume was added and resulting sample was loaded onto 15% nondenatureing polyacrylamide gel at 200 V for 2 hr. The gel was stained by Stains-All (Sigma).[8,9]

References.

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