Supporting Information

Synthetically Programmable DNA Binding Domains in Aggregates of DNA-Functionalized Gold Nanoparticles[†]

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Figure S1

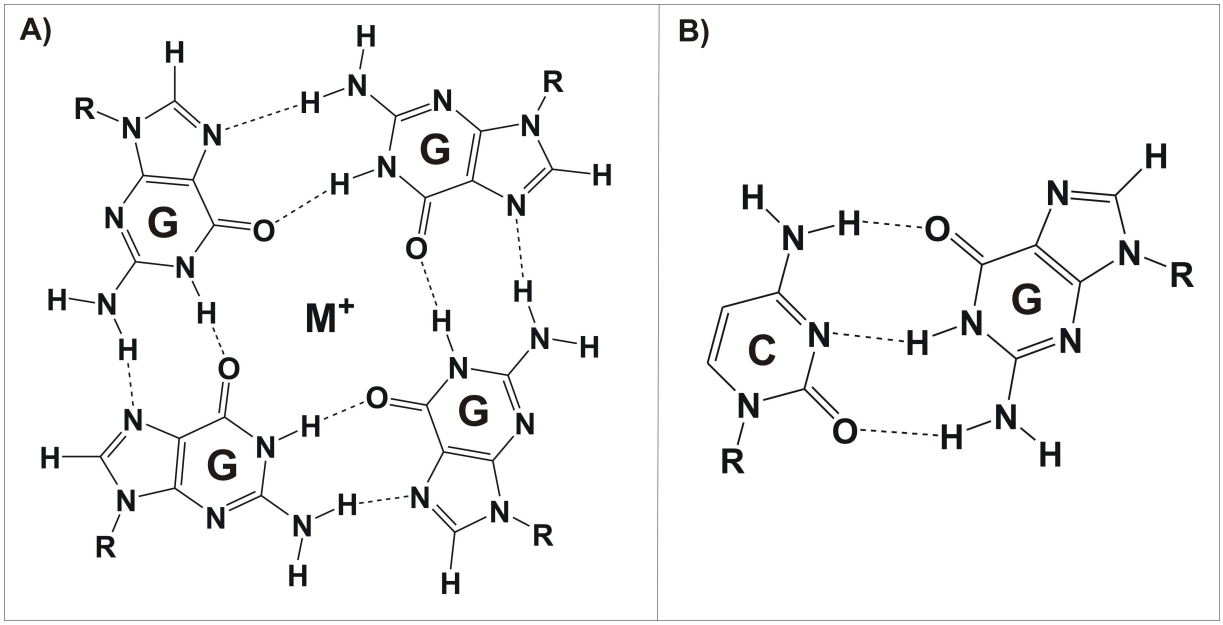

Figure S1. General structure of **A)** G-quadruplex and **B)** Watson-Crick binding interactions. Note that R denotes the connectivity of the base to the phosphate-sugar backbone and the dashed lines represent hydrogen bonding interactions. In **A)**, M^+ is a positively charged ion, typically K^+, Na^+, or Cs^+.

Figure S2

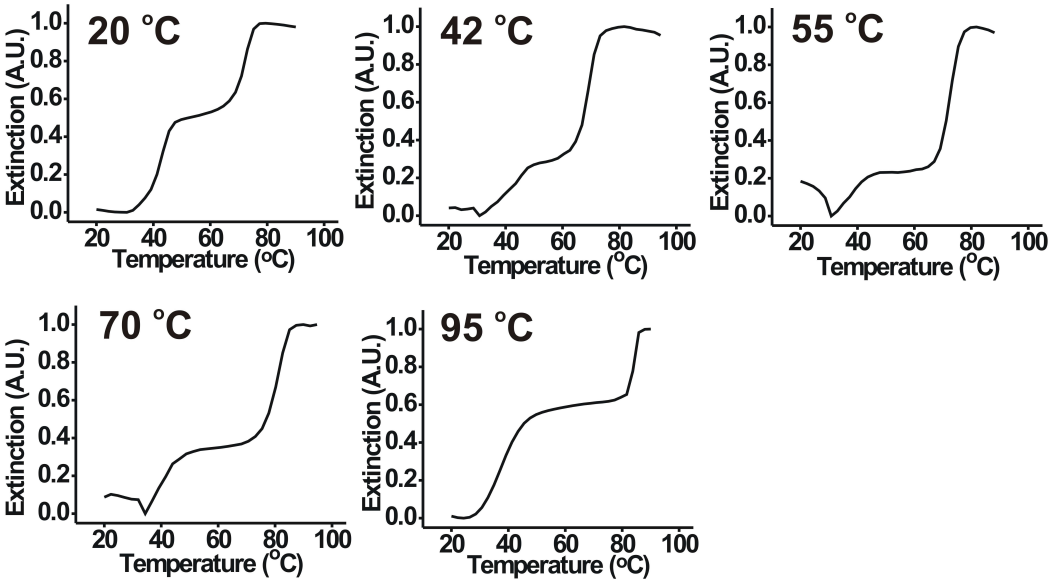

Figure S2. Normalized melting transitions (monitored at 260 nm) for aggregates of 60 nm DNA-Au NPs functionalized with A = TCCCC- and B = TGGGG- in 1.0 M NaCl, 10 mM sodium phosphate buffer, 0.01 % SDS annealed at the temperatures listed. These temperatures were chosen because they fall below transition 1 (20 °C), just below the melting temperature of transition 1 (42 °C), between transition 1 and 2 (55 °C), just below the melting temperature of transition 2 (70 °C), and above transition 2 (95 °C). Note that for the samples annealed at 42 °C, 55°C, and 70 °C transition 1 is comparatively smaller because after annealing all of the particles did not have time to rehybridize. These samples exhibit a small (less than 0.2 A.U. decrease in extinction below ~ 30 °C. These spectral features correspond to the continued hybridization of nanoparticles and the reorganization of the aggregate structure.[1]

References:

[1] R. Jin, G. Wu, C. A. Mirkin, G. C. Schatz, *J. Am. Chem. Soc.* **2003**, *125*, 1643.

Figure S3

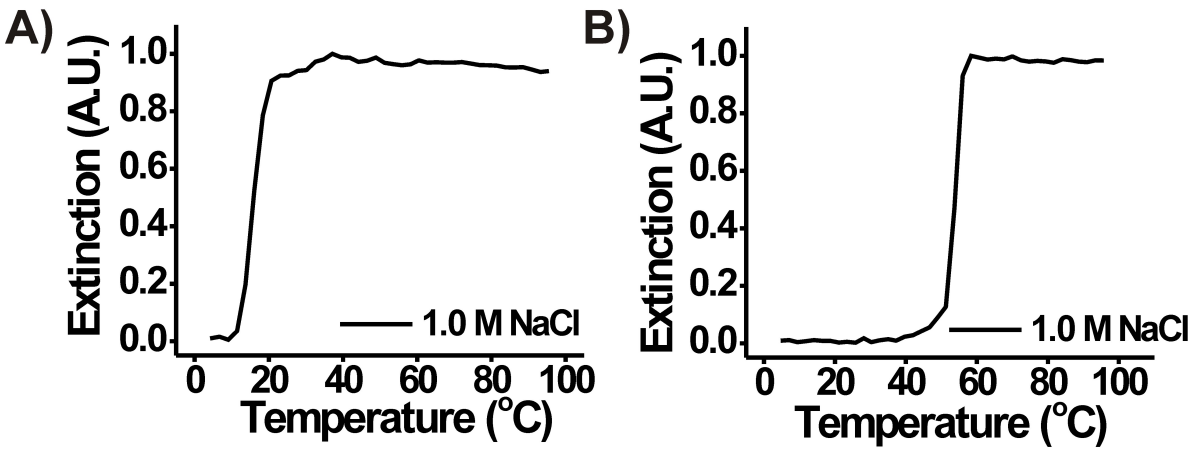

Figure S3. Normalized melting transitions (monitored at 260 nm) for aggregates of 60 nm DNA-Au NPs functionalized with **A)** A = B = TCG- and **B)** A = TCGC- and B = TGCG- in 1.0 M NaCl, 10 mM sodium phosphate buffer, 0.01 % SDS.

Figure S4

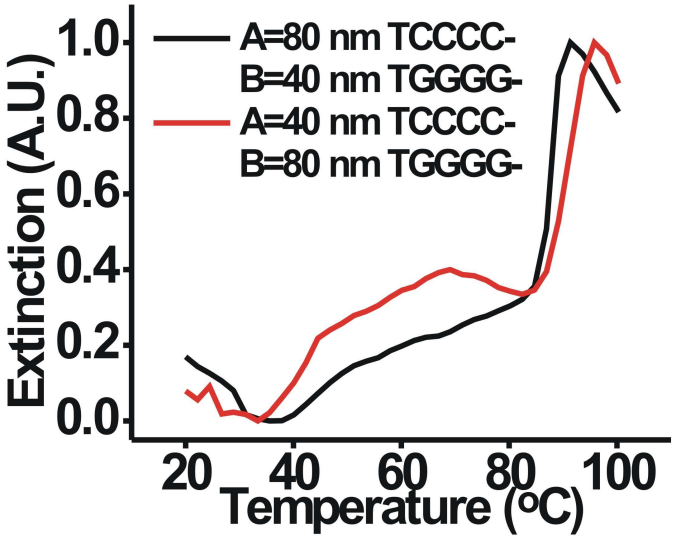

Figure S4. Normalized melting transitions (monitored at 560 nm) for aggregates of 40 nm DNA-Au NPs functionalized with TGGGG- and 80 nm DNA-Au NPs functionalized with TCCCC- (black trace) and 40 nm DNA-Au NPs functionalized with TCCCC- and 80 nm DNA-Au NPs functionalized with TGGGG- (red trace) in 0.4 M LiCl, 10 mM Li phosphate, 0.01 % LDS, 0.02 M KCl.

Figure S5

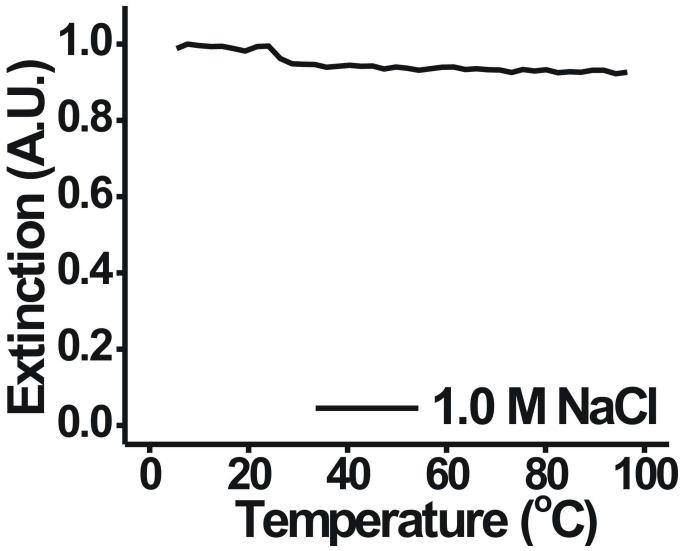

Figure S5. Normalized temperature profile (monitored at 260 nm) for 60 nm DNA-Au NPs functionalized with a control poly-T DNA sequence in 1.0 M NaCl, 10 mM sodium phosphate buffer, 0.01 % SDS.

Table S1. List of DNA sequences.

Name	Oligonucleotide Sequence
TCG-	5′ – TCG TTT TTT TTT TTT TTT TTT TTT – $(CH_2)_3$ – SH – 3′
TCGC-	5′ – TCG CTT TTT TTT TTT TTT TTT TTT – $(CH_2)_3$ – SH – 3′
TGCG-	5′ – TGC GTT TTT TTT TTT TTT TTT TTT – $(CH_2)_3$ – SH – 3′