Electronic Supplementary Material (ESI) for Biomaterials Science.

Supporting Information

Quantitative Measurements of Thermodynamics and Kinetics of Polythiophene-DNA Complex Formation in DNA Detection

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Submitted to *Biomaterials Science*

Table S1: Summary of DNA sequences used in this study:

Name	Sequence	Description
X1	5'TAA CAA TAA TCC CTC	DNA probe
X1'	5'-TAA CAA TAA TCC CTC A_{20}-C_3-S-S-C_3-OH	DNA probe to bind on silica nanoparticles
Y1	5'-GAG GGA TTA TTG TTA	DNA Complementary to ***X1, X1'***

Calculation of surface density of immobilized polymer-ssDNA duplex on silica nanoparticles:

Volume of 100-nm silica nanoparticle, $V = (\pi/6)*D^3 = (3.14/6)*(10^{-5}\ \text{cm})^3 = 5.2*10^{-16}\text{cm}^3$;

Surface area of 100-nm silica nanoparticle, $S = \pi D^2 = 3.14*(10^{-5}\ \text{cm})^2 = 3.14*10^{-10}\text{cm}^2$;

Weight of silica nanoparticle, $W = \rho*V = (1.96\ \text{g/mL})*(5.2*10^{-16}\text{cm}^3) = 1.02*10^{-15}\text{g}$;

For 100 μL of 15mg/mL particle solution, total weight of particle, W_t:

$$W_t = (100*10^{-6}\ \text{L})*(15\ \text{mg/mL}) = 1.5*10^{-3}\ \text{g};$$

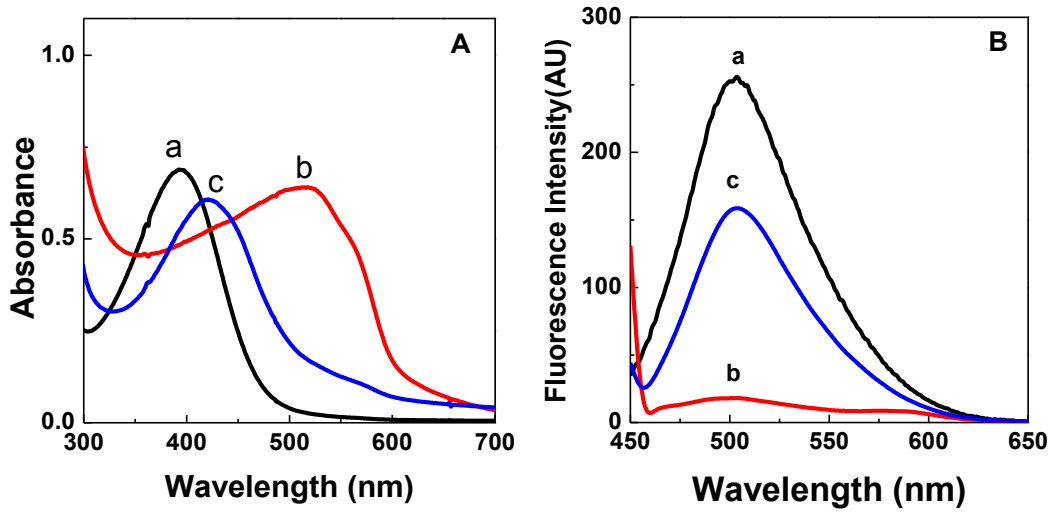
Number of particles in solution, $N = W_t/W = (1.5*10^{-3}\ \text{g})/(1.02*10^{-15}\text{g}) = 1.5*10^{12}$;

Total surface area of particles, $S_t = N*S = (1.5*10^{12})*(3.14*10^{-10}\text{cm}^2) = 471\ \text{cm}^2$;

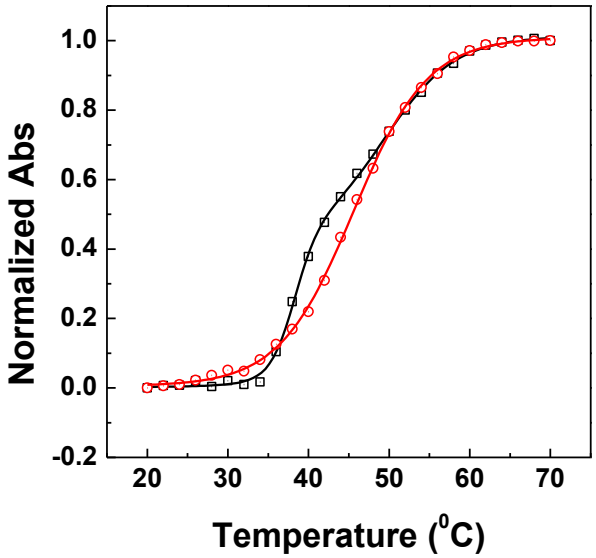
Surface density of immobilized polymer-ssDNA duplex on particles, Γ:

$$\Gamma = (\text{mole of duplex})/S_t = (100*10^{-6}\ \text{L})*(16*10^{-6}\ \text{mol/L})/(471\text{cm}^2)$$

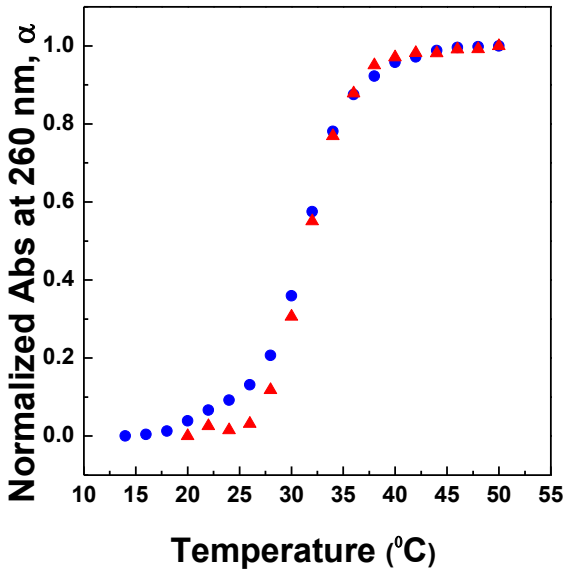
$$\approx 3*10^{-12}\ \text{mol/cm}^2 = 3\ \text{pmol/cm}^2.$$



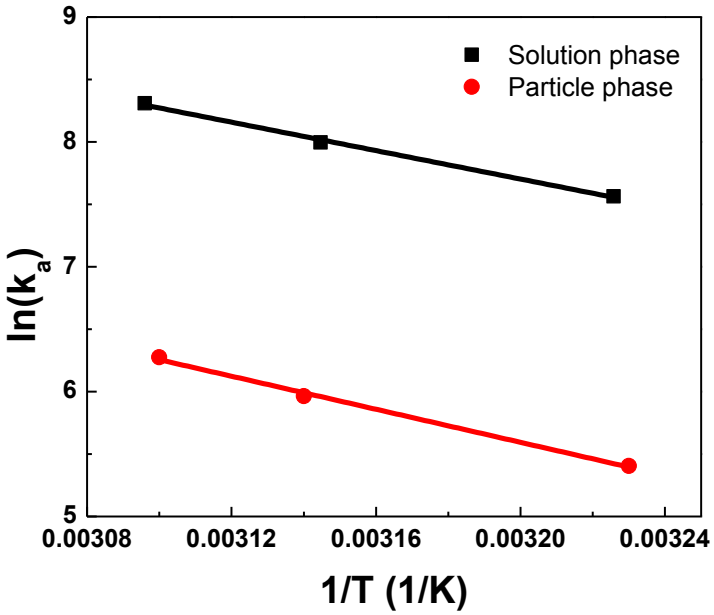
Supporting Figure 1. **(A)** Absorbance and (**B**) fluorescence emission profiles of conjugated polymer-DNA complexes: **(a)** free polymer, **(b)** polymer/ssDNA duplexes, and **(c)** polymer/dsDNA triplexes.



Supporting Figure 2. Melting curves of the polymer-ssDNA duplexes in 10 mM PB buffer monitored at 260 nm (black squares) and 500 nm (red circles). The corresponding solid lines are the best fit of experimental data.



Supporting Figure 3. The melting curves of dsDNA in solution without (red triangles) or with (blue circles) the extra A_{20} spacer. The presence of A_{20} as the spacer only slightly changed the melting temperature of dsDNA at the absence polymer with the calculated K value increased from 2.2 x 10^{-8} to 4.3 x 10^{-8}. No stability change was observed for the polymer-dsDNA system, primarily due to the much higher temperature needed to dissociate polymer-dsDNA triplexes that no polymer-ssA20, if any, would be able to survive.



Supporting Figure 4. Arrhenius plots for conjugated polymer-bound DNA hybridization in solution phase and on particle phase. Association rate constants were determined from the fitting curves recorded at different temperatures.