Visible Light-Induced Charge injection and migration in self-assembled Carbon Dot-DNA-Carbon Dot Nano-dumbbell obtained through controlled stoichiometric conjugation

Saptarshi Mandal, Prolay Das*

Department of Chemistry, Indian Institute of Technology Patna, India

Supplementary Information

Materials

Desalted synthetic oligonucleotides (5′-PO_4^{2-}-ATATGGATATGGATAT-3′ and 5′-PO_4^{2-}-ATATCCATATCCATAT-3′) were purchased from Sigma-Aldrich custom oligo service. SYBR Gold was acquired from Invitrogen. 1,4-diaminoanthraquinone (1,4-DAAQ), acrylamide, N,N'-methylenebisacrylamide, ammonium persulfate, N,N,N',N'-tetramethylethylenediamine (TEMED), tetrabutylammonium hexafluorophosphate ($[Bu_4N]PF_6$), 1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC.HCl) were obtained from TCI Chemicals India Pvt. Ltd. Urea, formamide, dimethylformamide (DMF), acetonitrile (ACN), 2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid (HEPES), sodium phosphate dibasic (Na_2HPO_4) and monobasic (NaH_2PO_4), tris-base, taurine, ethylenediaminetetraacetic acid, imidazole, potassium bromide were procured from Merck, India. Ultrapure water from Milli-Q was used as solvent unless specified.

Estimation of amines on CD surface

Amine functional groups on the CD surface were estimated approximately through Ninhydrin assay. First, a standard curve of absorbance vs. concentration of $–NH_2$ functional groups was generated by performing a Ninhydrin assay of Glycine with known concentrations. Then the CD solution was reacted with Ninhydrin, and the absorbance was measured. The amount of surface $–NH_2$ groups was estimated from the following standard curve generated equation:

$Y = 948 \times 10^{-6} X$, where Y is the absorbance value, and X is the $–NH_2$ concentration in nmol.

The concentration $–NH_2$ functional groups were calculated as 8 nmol/μL of CD stock solution. We diluted the stock CD solution with water to 0.8 nmol/μL for conjugation with the DNA strands.

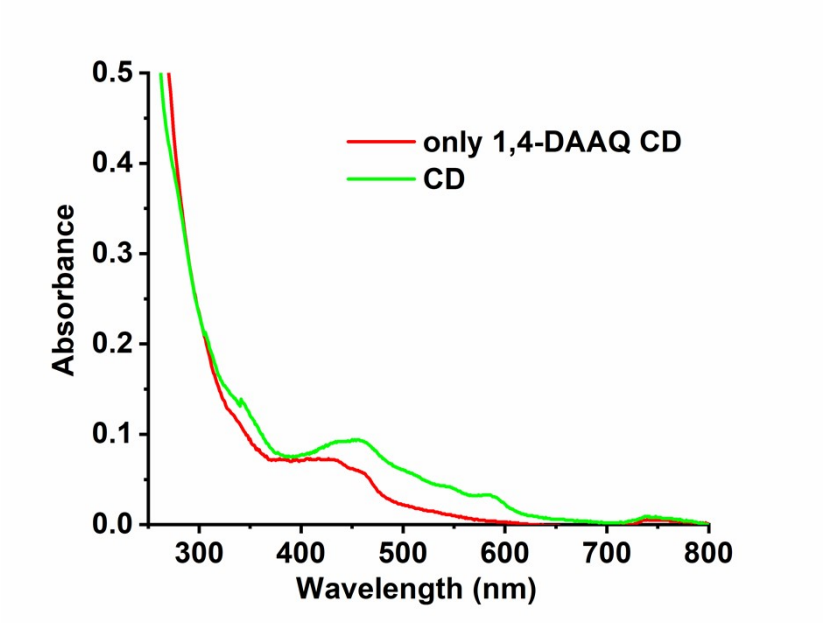

Figure S1. UV-Vis absorption spectra of only 1,4-DAAQ CD, and 1,4-DAAQ and glyoxal-based CD.

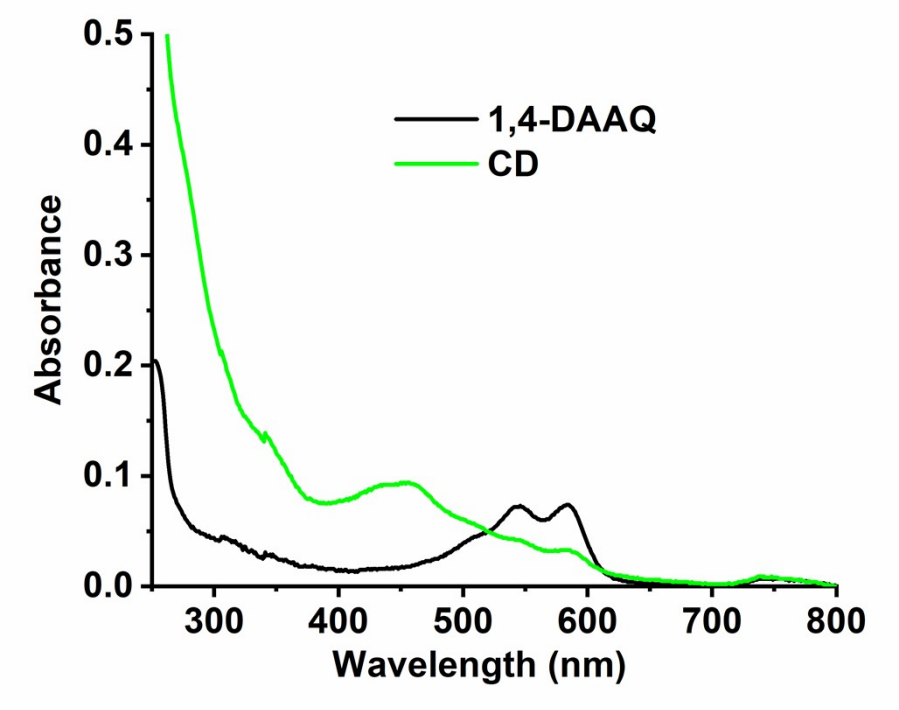

Figure S2. UV-vis absorption spectra of the CD and 1,4-DAAQ.

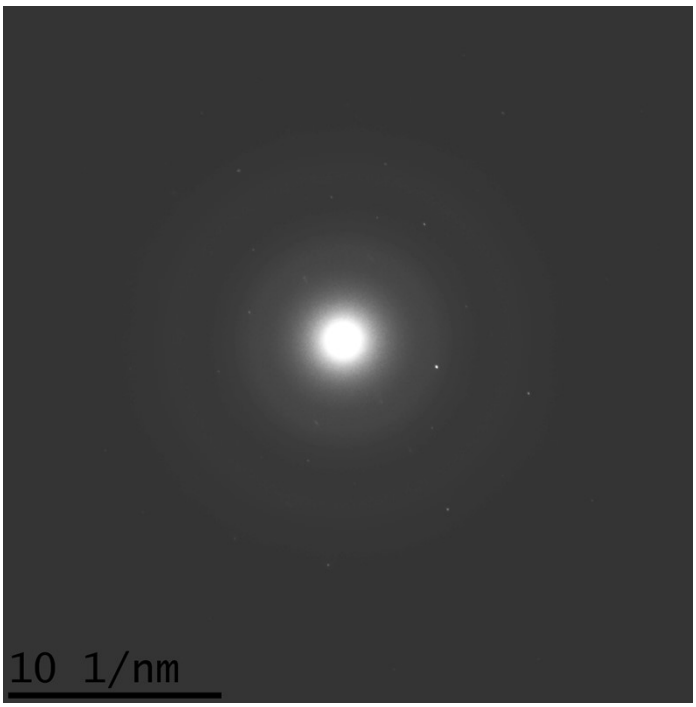

Figure S3. SAED pattern of the CD revealing amorphous or poor crystallinity of the CD.

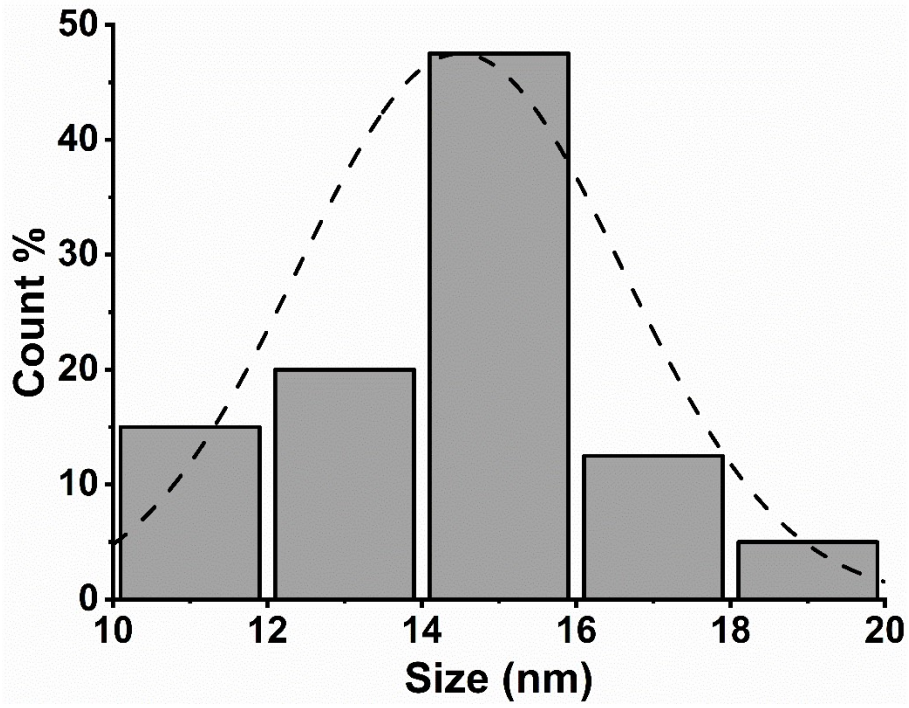

Figure S4. Size distribution of CD.

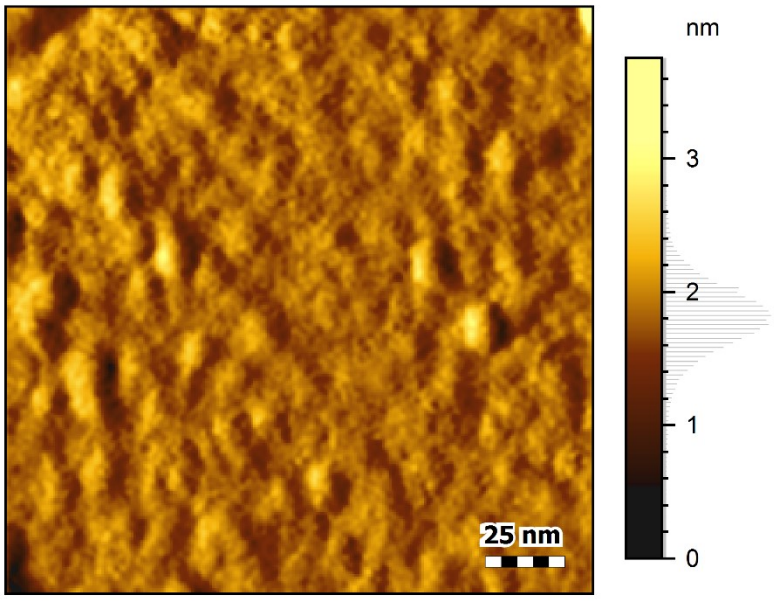

Figure S5. AFM image of the CD revealed a near-spherical shape.

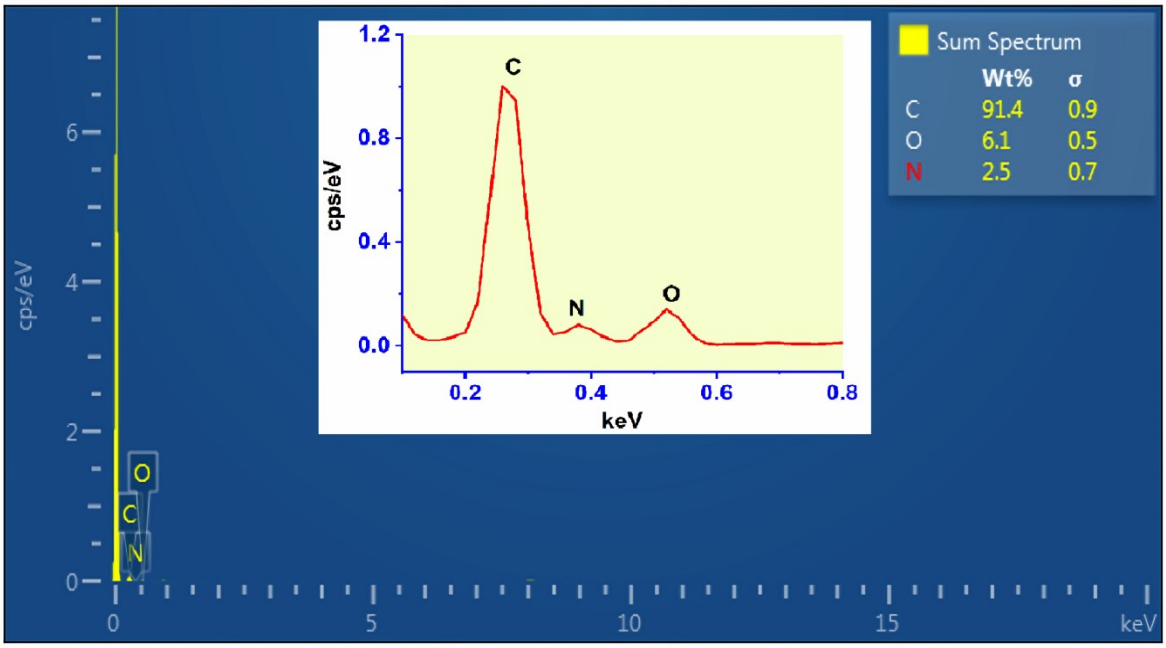

Figure S6. EDS spectra of the CD showing the presence of C, N, and O in the elemental composition of the CD.

Table S1. Elemental calculation of CD from EDS.

Element	Line Type	k Factor	k Factor type	Absorption Correction	Wt%	Wt% Sigma	Atomic %
C	K series	3.115	Theoretical	1.00	91.43	0.88	93.17
N	K series	1.807	Theoretical	1.00	2.51	0.72	2.20
O	K series	1.455	Theoretical	1.00	6.06	0.55	4.64
Total:					100.00		100.00

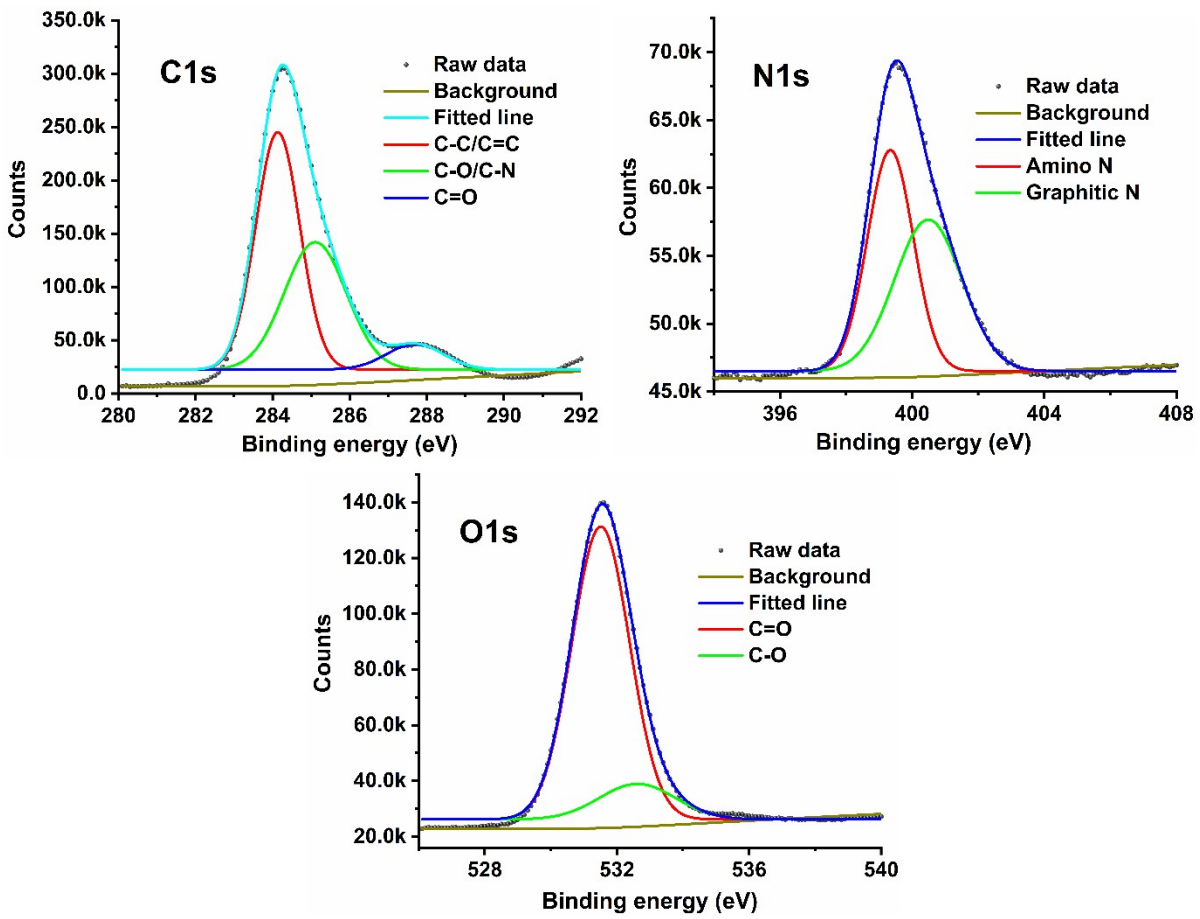

Figure S7: High resolution C1s, N1s and O1s XPS spectra of the CD.

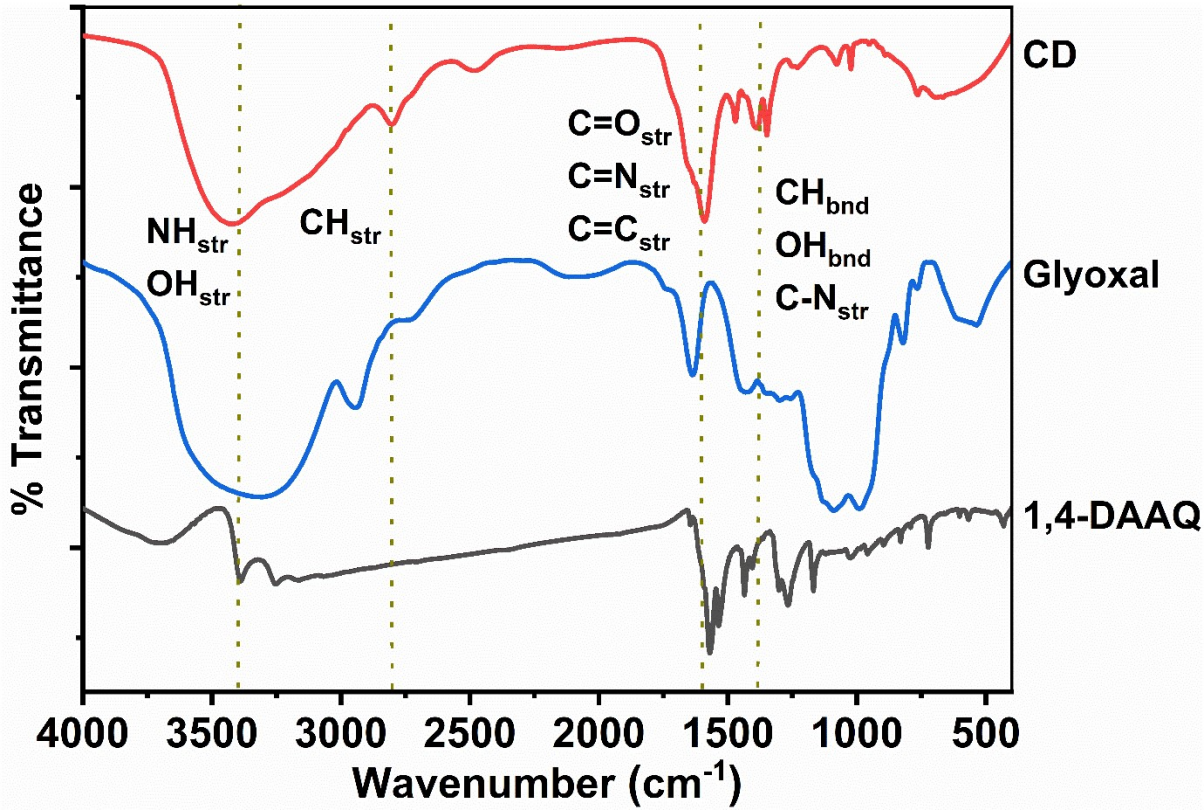

Figure S8. FTIR spectra of the CD along with the precursors 1,4-DAAQ and glyoxal. str: stretching, bnd: bending

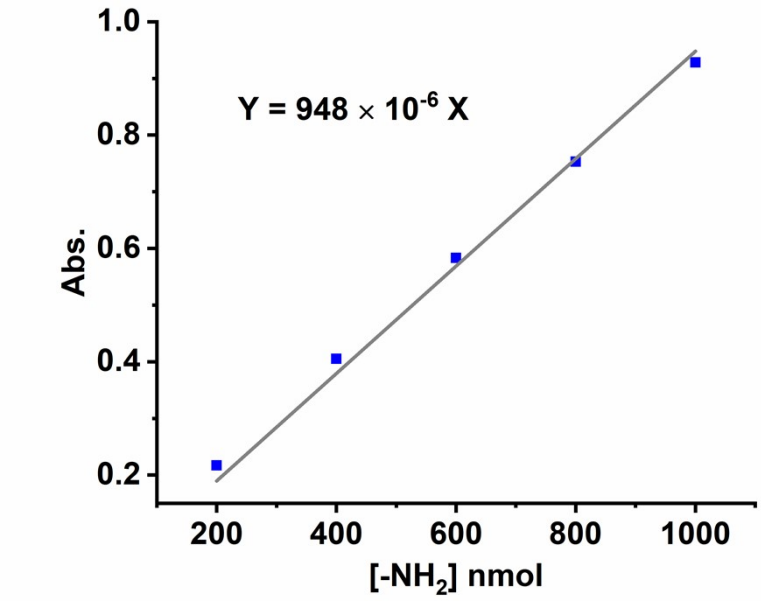

Figure S9. Ninhydrin assay standard curve.

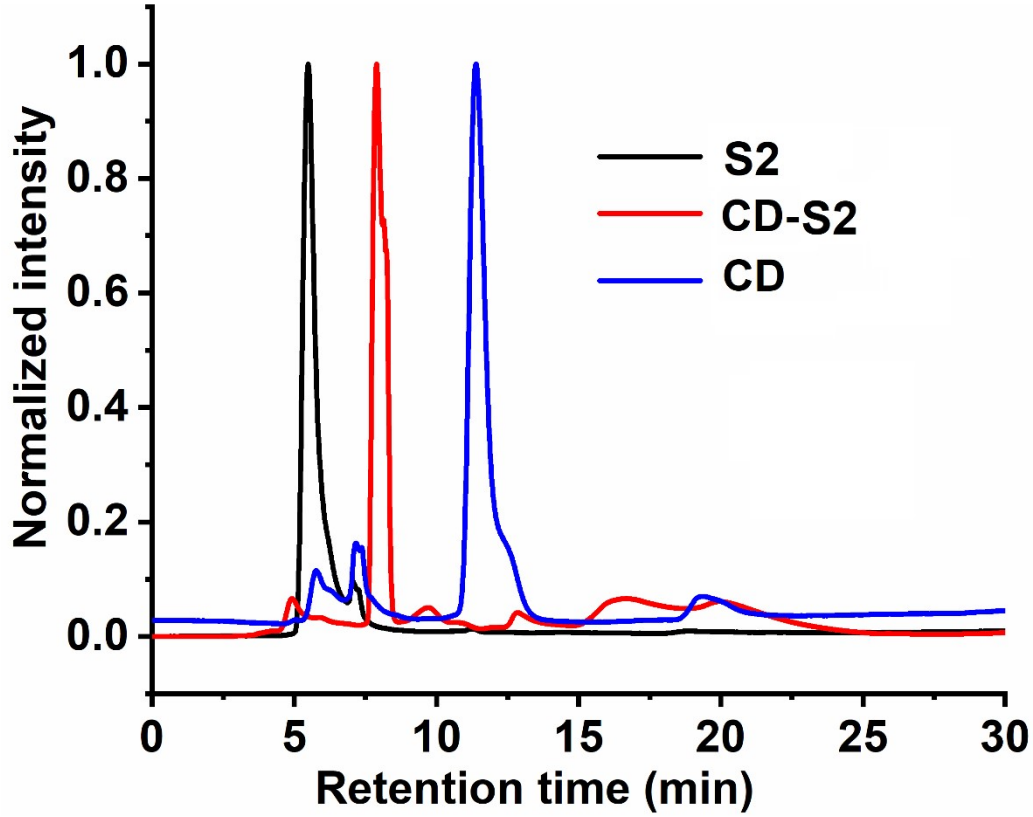

Figure S10. HPLC profile for CD-S2 conjugation.

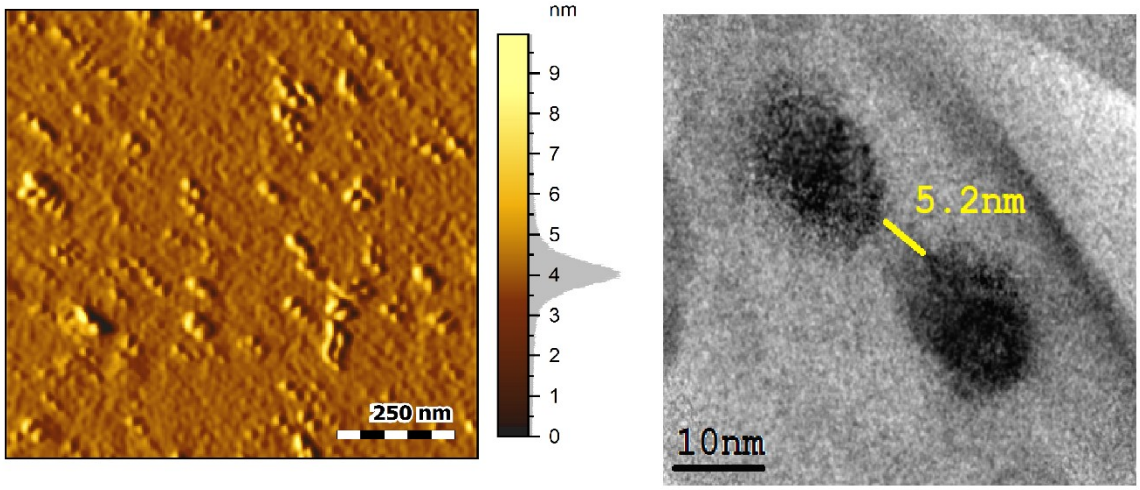

Figure S11. AFM and TEM images of the CD-S1-S2-CD dumbbell

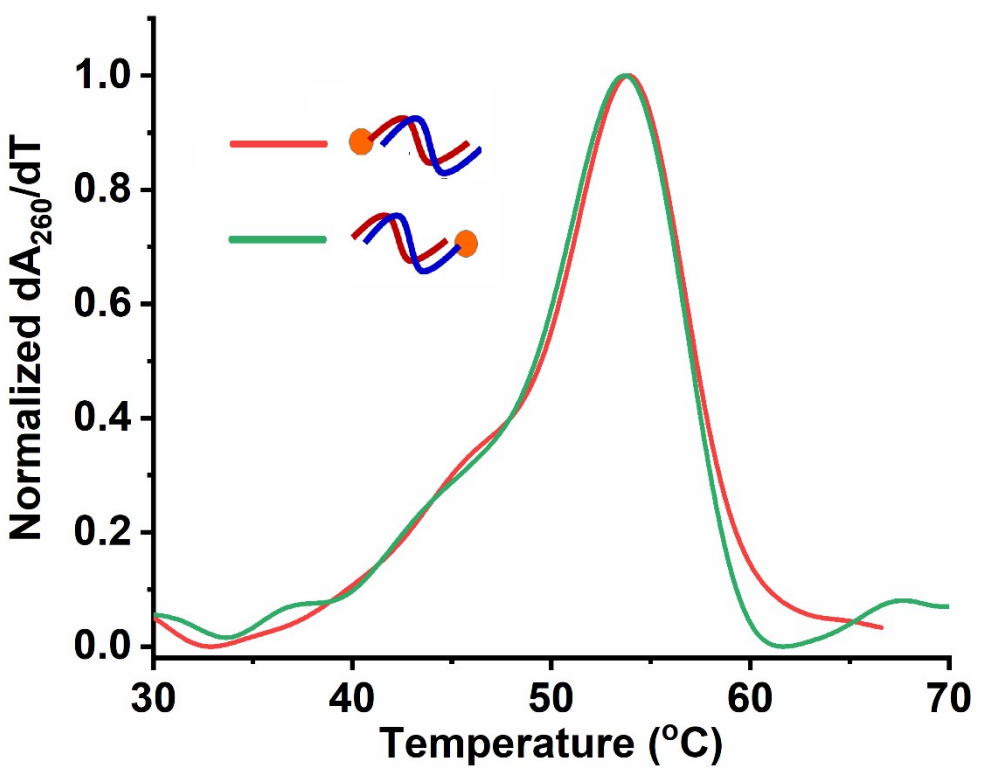

Figure S12. Thermal melting curves of CD-S1-S2 and S1-S2-CD.

Table S2. T_m value of DNA hybridized systems.

Hybridized system				
T_m value (°C)	54.5	53.9	53.8	52.5

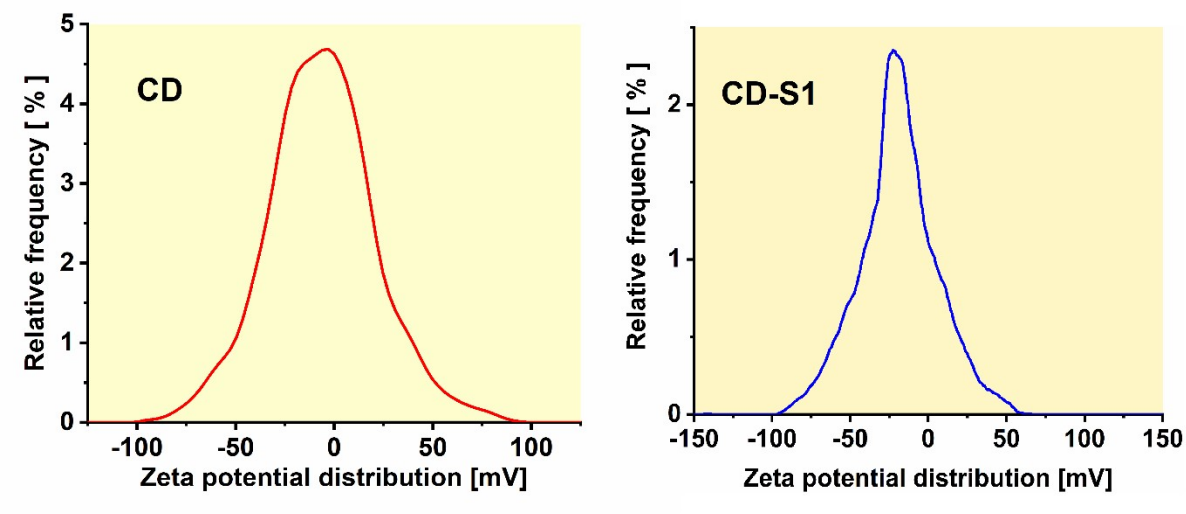

Figure S13. Zeta potential of the CD and CD-S1 conjugate, revealing a negative zeta potential for both the samples.

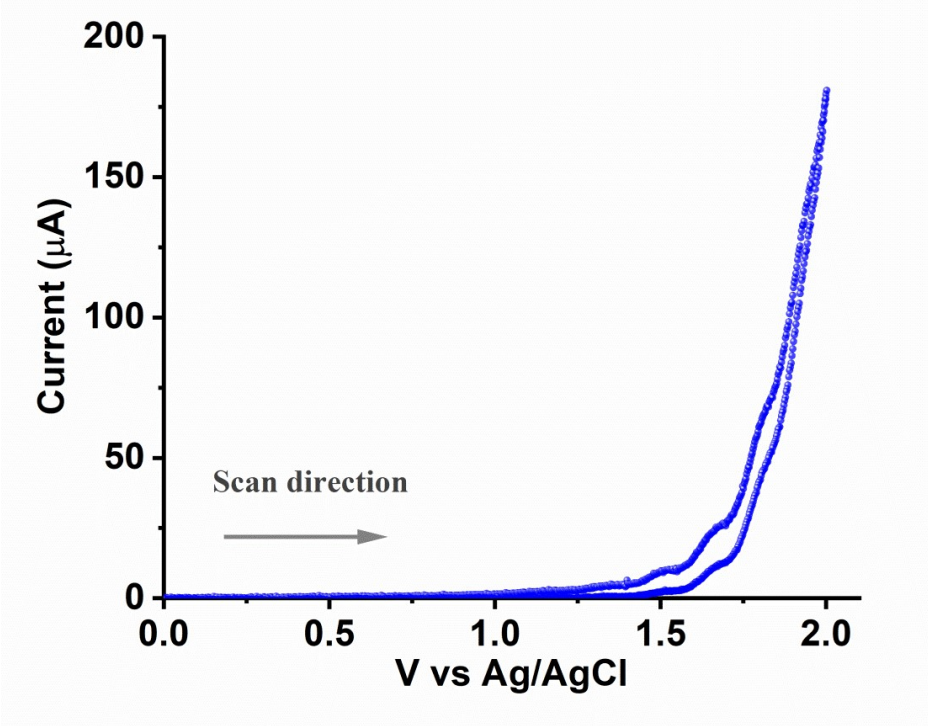

Figure S14. Cyclic voltammogram of the CD in acetonitrile at scan rate 30 mV/s.

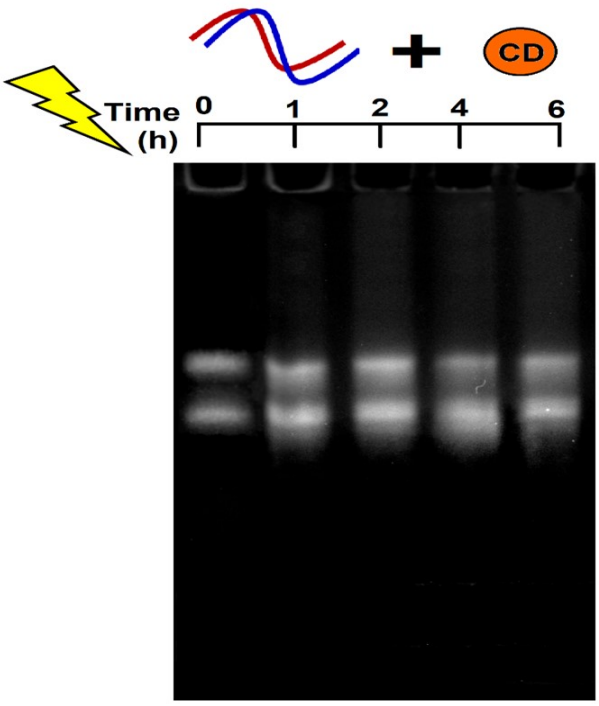

Figure S15. S1-S2 and CD physical mixture with varying irradiation time with 100W tungsten bulb.

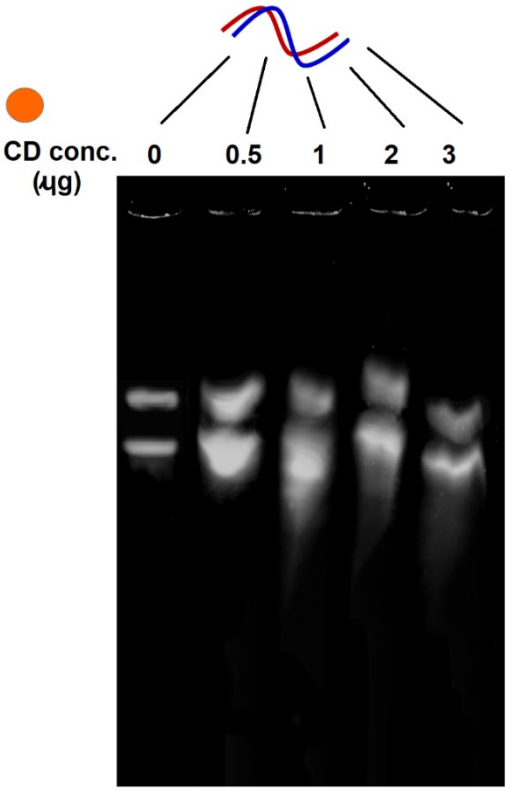

Figure S16. S1-S2 CD physical mixture with increasing CD concentration irradiated under 100W tungsten bulb.

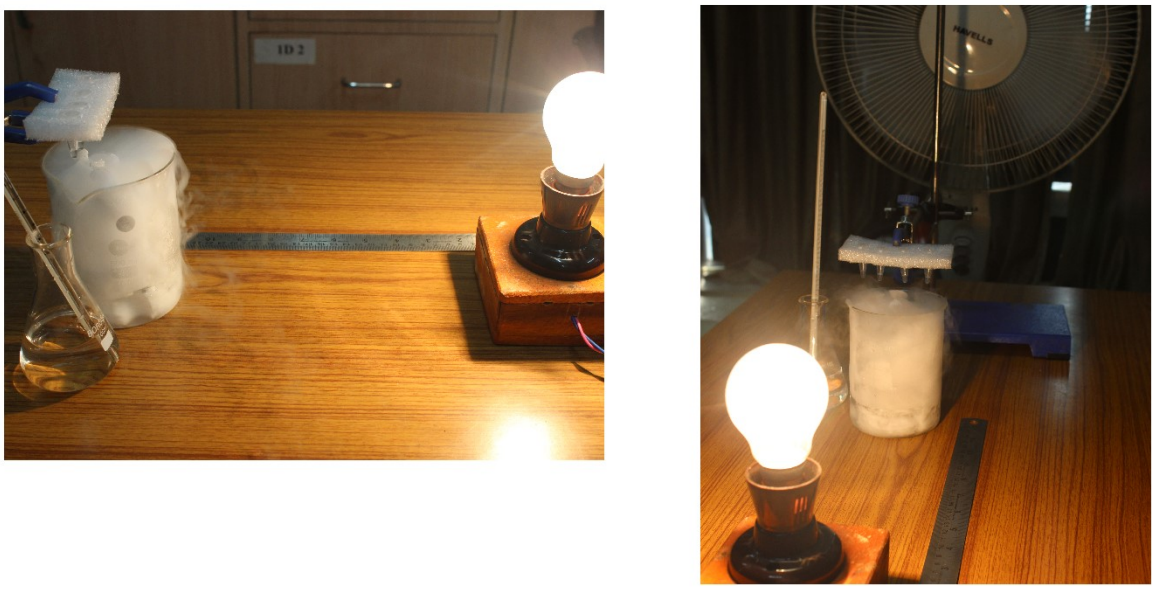

Figure S17. Experimental set up for irradiation of nano-assemblies with visible light from a tungsten source

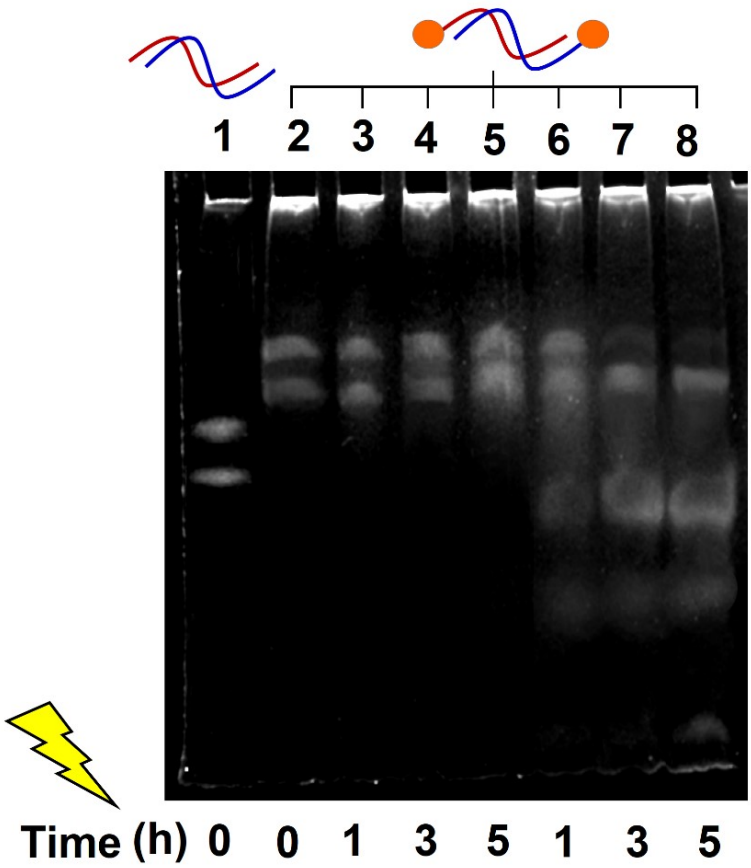

Figure S18. CD-DNA dumbbell systems with varying irradiation time under 28W white tube light and 100W tungsten bulb.

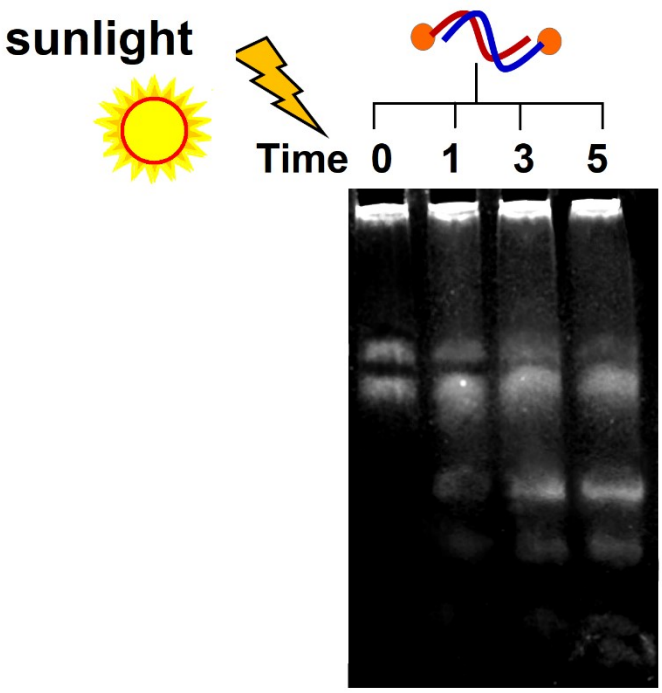

Figure S19. CD-S1-S2-CD strand connected CD hybridized DNA with varying irradiation time under natural sunlight 1 3 5 hours