# On the Molecular Origin of Photoluminescence of Nonblinking Carbon Dot

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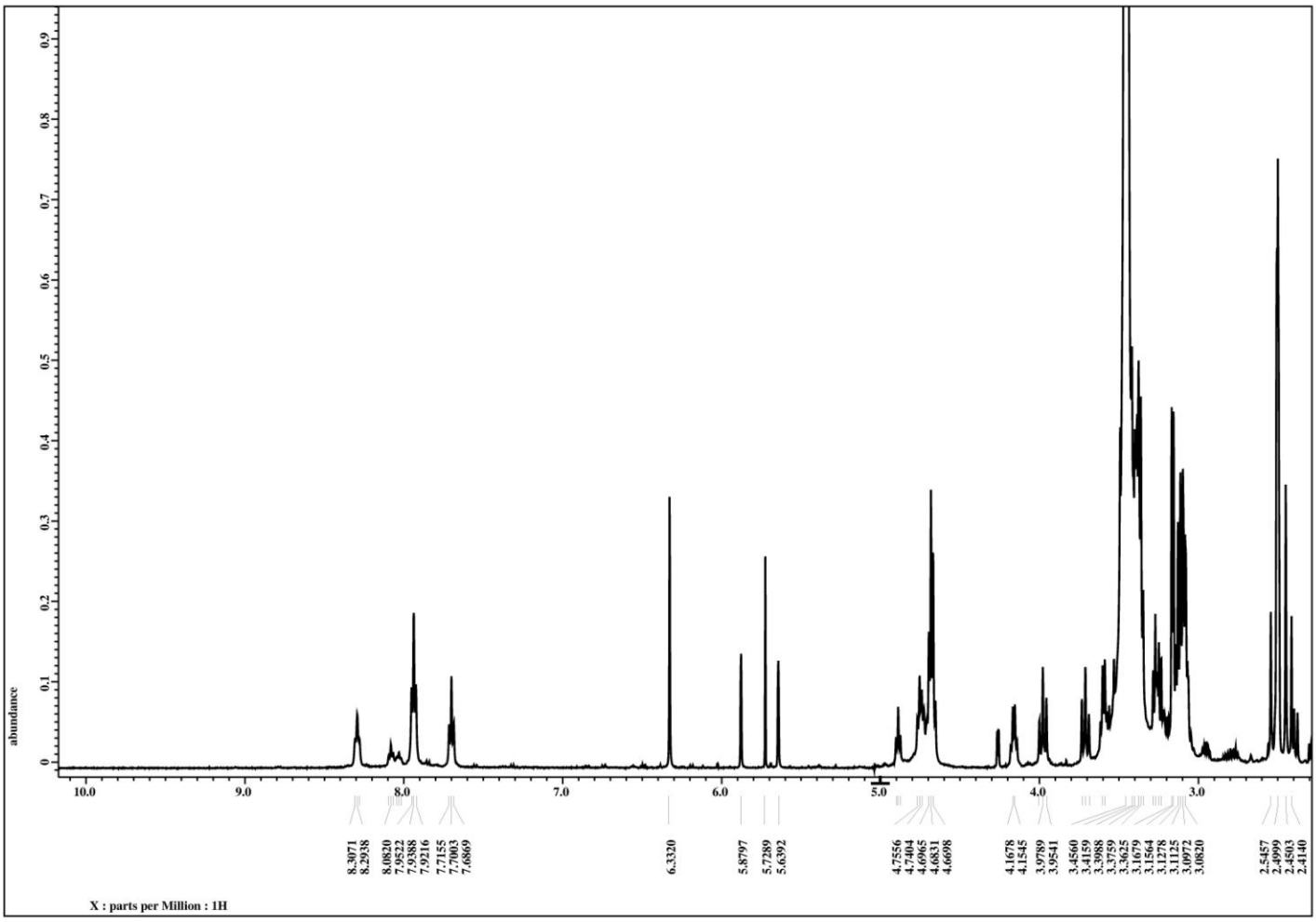



**Figure S1**. $^{1}H$ NMR spectrum of CD in DMSO-$d_6$.

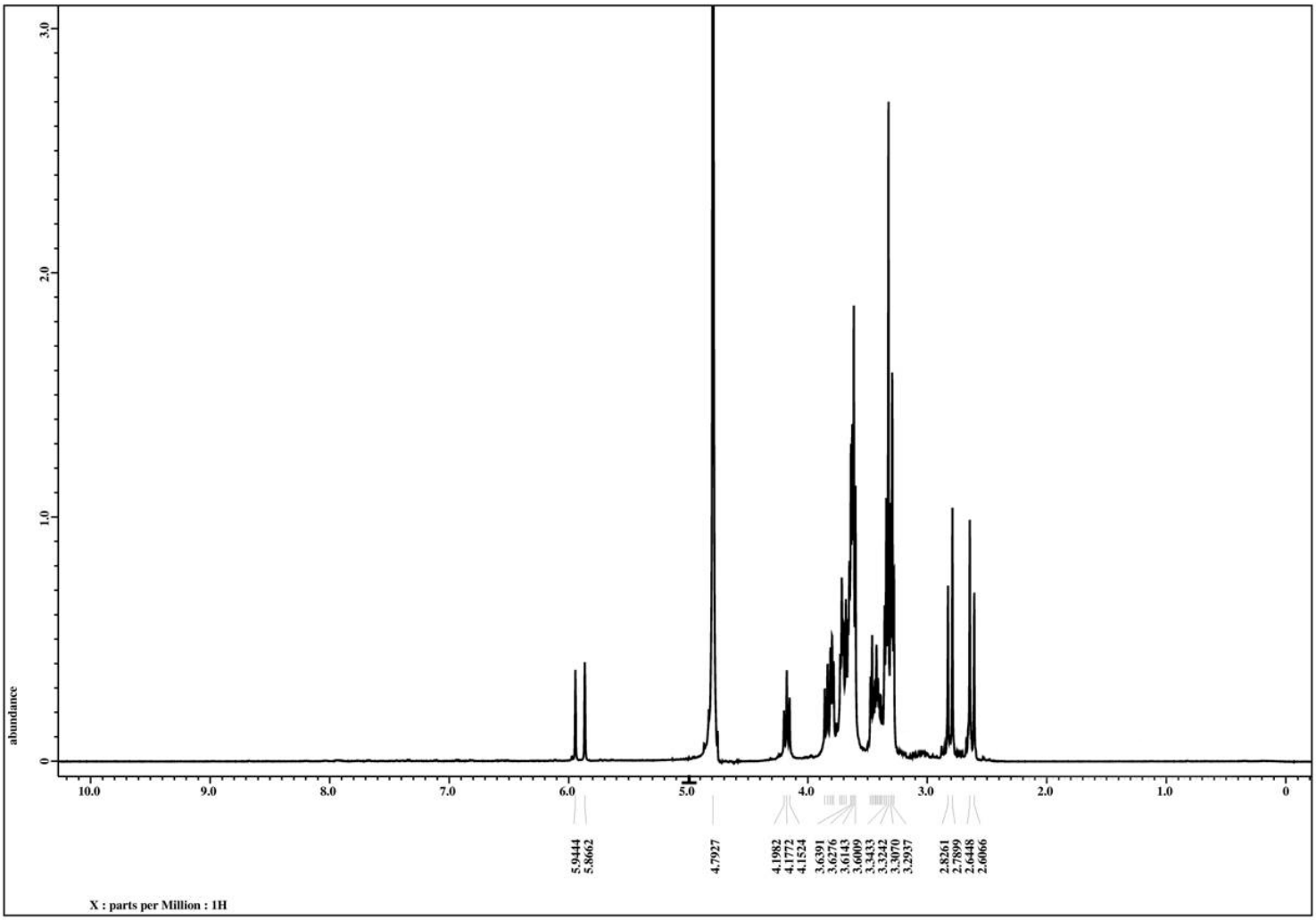
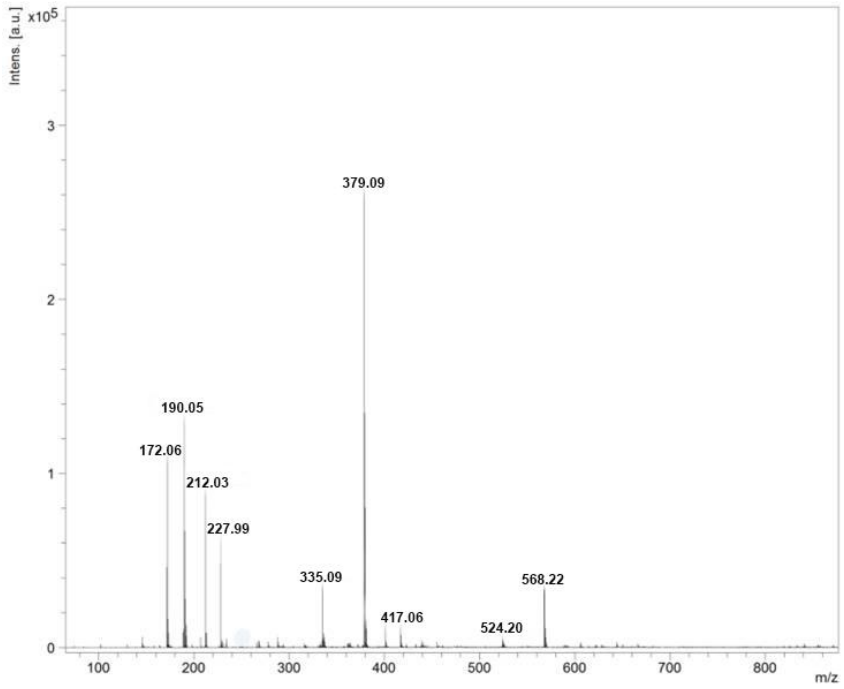



**Figure S2**. $^{1}H$ NMR spectrum of CD in $D_2O$.

**(a)**




**(b)**

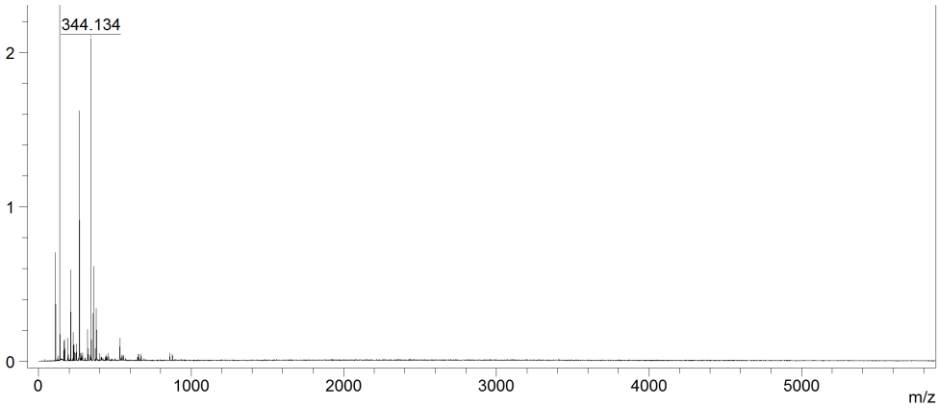



**Figure S3**. MALDI mass spectrum of CHCA Matrix (a), MALDI mass spectrum of CDs with CHCA matrix (b).

**Table S1. m/z values in MALDI mass**

| | m/z values |
|---|---|
| CHCA matrix | 172.06, 190.05, 212.03, 227.99, 335.09, 379.09, 417.06, 524.20, 568.22 |
| CDs with CHCA matrix | 172.06, 212.03, 227.99, **249.99**, **268.11**, **286.10**, **322.16**, **344.13**, **360.11**, 379.09, 568.20 |

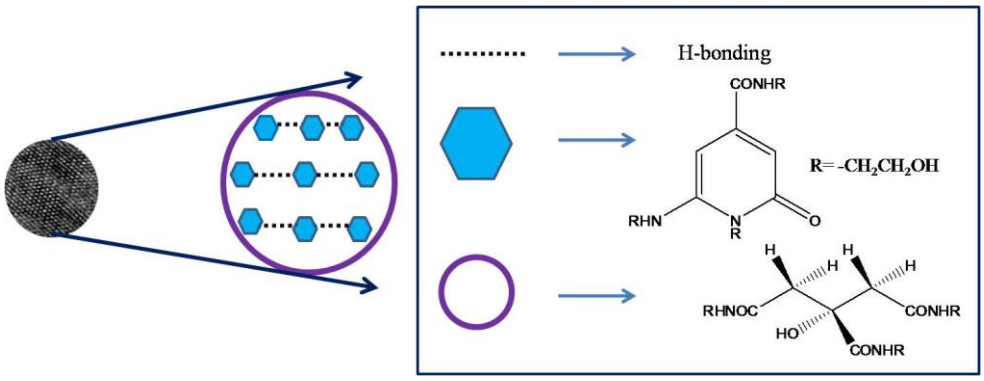



**Figure S4**. Formation of CD by stacking of fluorophores.

## AFM experimental details and image.

The morphology of carbon dot was investigated by atomic force microscopy. Atomic force microscopy was carried on NT-MDT (model no. AP-0100) in semicontact mode. The carbon dot was dissolved in methanol and drop casted on a microscopic glass coverslip.

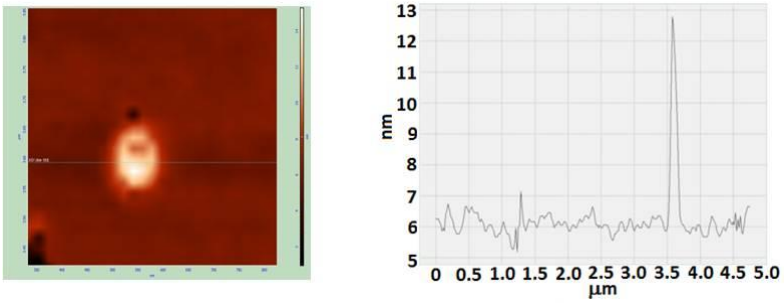



**Figure S5**. AFM image and its corresponding size of CD.

**Figure S6**.Inverted round-bottomed flask showing gel nature of CD.

## Computational calculation of 2-pyridone derivative.

The geometry of the molecule has been optimized by density function theory (DFT) using Gaussian 09 software [S1]. All the calculations were performed using B3LYP functional and 6-31G basis set for all the atoms. Default criteria for geometry optimization were used in each case.

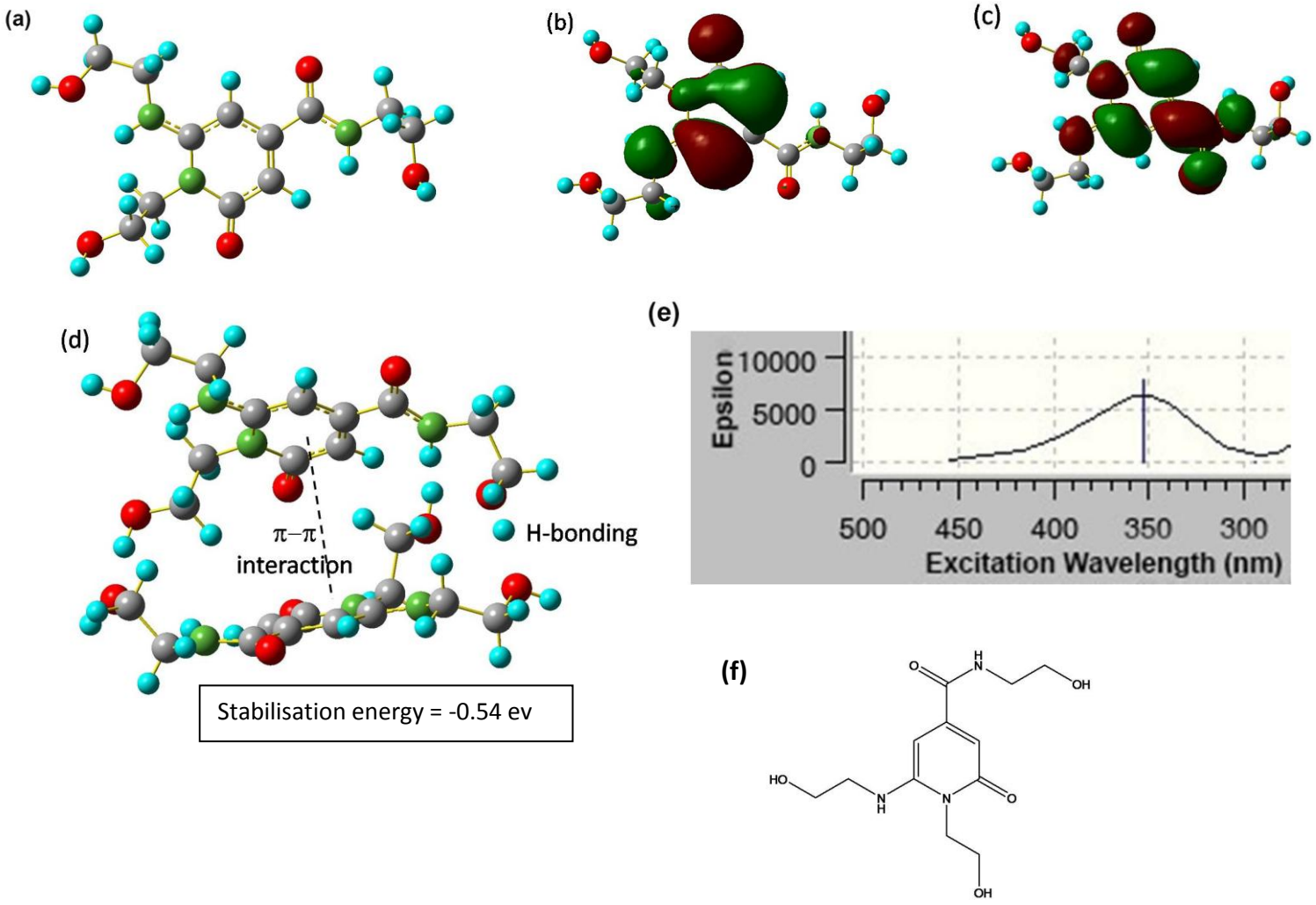



**Figure S7**. Geometry optimized structure (a), orbital picture of HOMO (b), LUMO (c) of 2-pyridone derivative. Stabilisation due to π-π interaction and H-bonding (stabilisation energy = -0.54 ev) has been shown in between two 2-pyridone derivatives (d). Computational UV-VIS spectrum of 2-pyridone derivative (e). Structure of 2-pyridone derivatives (f).

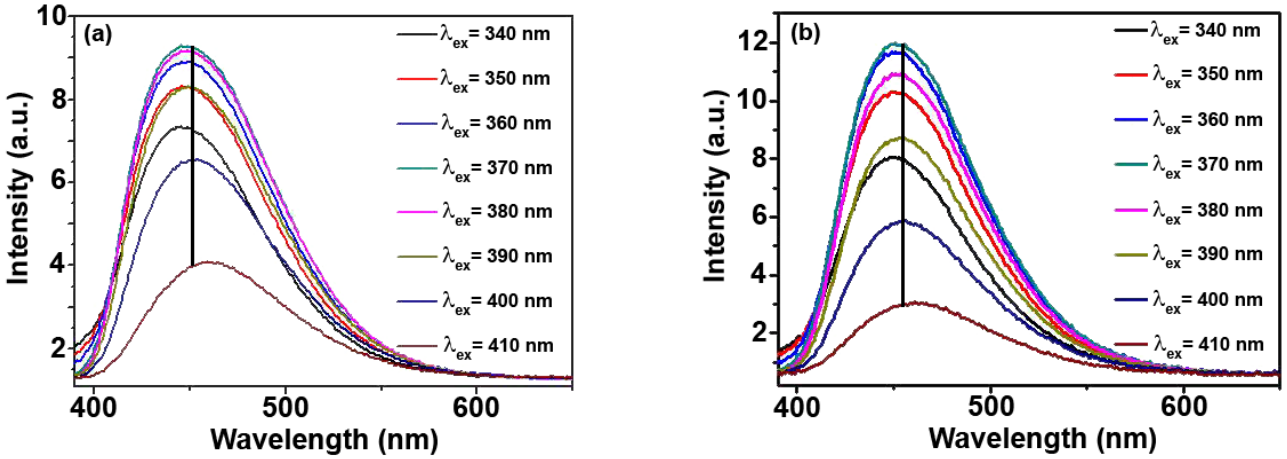



**Figure S8**. Emission behavior of CD in acetonitrile (a) and methanol (b).

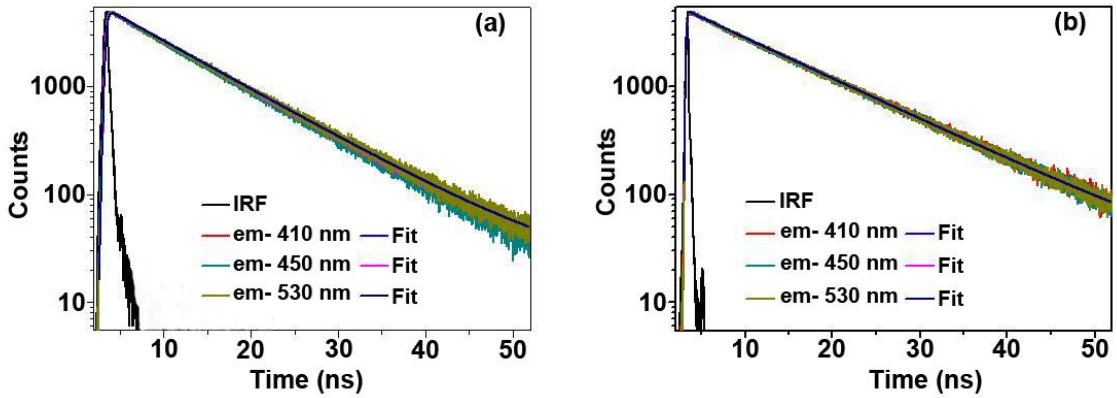



**Figure S9**. TCSPC decay of CD in acetonitrile (a) and methanol (b).

## Photostability experiment:

Procedure for photostability measurement:

For photostability measurement 25 mL stock solutions of carbon dot (in water), CdSe QD (in toluene), and CdSe/CdS QD (in toluene) were kept in three different glass vials (volume = 30 mL) and put in a UV chamber. Absorbance of each solution of carbon dot, CdSe QD and CdSe/CdS QD were kept in between 0.18 to 0.20 at the irradiation wavelength (360 nm) (see figure below). Three stock solutions were continuously irradiated with two 360 nm 8 W each UV lamps. The distance between UV lamp and the top of each glass vial was 10 cm.

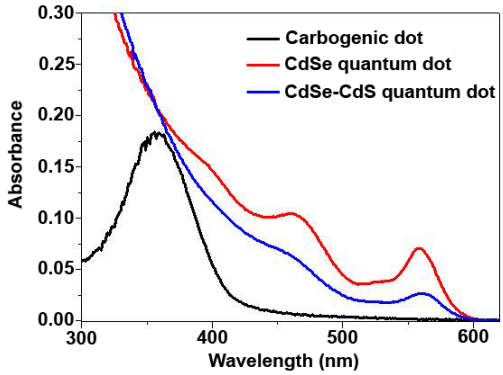



**Figure S10**. Absorption spectra of carbon dot, CdSe QD, and CdSe/CdS core-shell QD.

Synthesis of QD.

CdSe core was synthesized following a literature procedure using 'hot injection' method [S2]. TOPO was used as a ligand. CdSe QDs were purified by centrifugation and decantation and then dispersed in toluene for further processing. CdSe/CdS core/shell QDs were prepared by SILAR (Successive Ion Layer Adhesion and Reaction) technique following a literature procedure [S3,S4]. Oleic acid was used as a ligand. Both the CdSe-core and CdSe/CdS core/shell QDs were synthesized in Schlenk line setup to maintain standard air free atmosphere. All chemicals required for the synthesis of QD were procured from Sigma-Aldrich.

## pH dependent experiment:

All the solutions (from pH 2 to pH 12) were prepared and checked by using a bench top pH meter (SESHIN, ECM-710). A fixed amount of CD was dissolved in all pH solutions (~ 4 μg in 2.5 mL). Absorption spectra were recorded in Carry 300 Bio UV-VIS spectrophotometer.

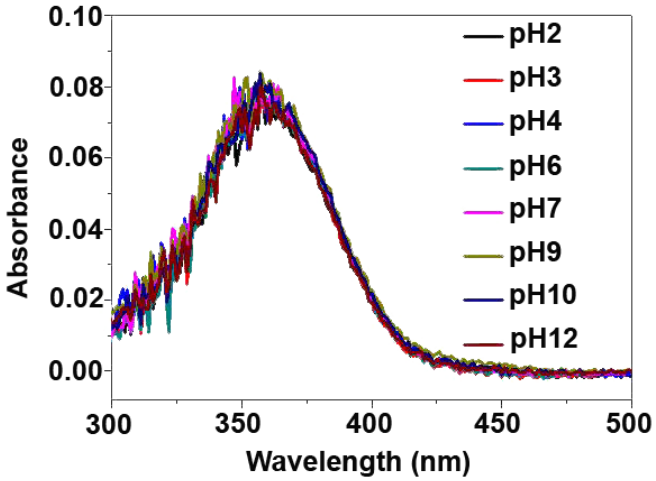



**Figure S11**. Absorption spectra of CD at different pH.

## Single particle movie:

A movie showing the gradual decrease of PL intensity of CD at the single particle level.


Movie_Final.avi

# References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[S2] Aldana, J.; Wang, Y. A.; Peng , X. G. Photochemical Instability of CdSe Nanocrystals Coated by Hydrophilic Thiols. *J. Am. Chem. Soc.* **2001**, *123*, 8844-8850.

[S3] Li, J. J.; Wang,Y. A.; Guo,W. Z.; Keay,J. C.; Mishima,T. D.; Johnson,M. B.; Peng, X. G. Large-Scale Synthesis of Nearly Monodisperse CdSe/CdS Core/Shell Nanocrystals Using Air-Stable Reagents via Successive Ion Layer Adsorption and Reaction. *J. Am. Chem. Soc.* **2003**, *125***,** 12567-12575.

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