Supporting Information

A self-assembled CdSe QD-organogel hybrid: Photophysical and thermoresponsive properties

Sayantan Chatterjee*, Balamurugan Kuppan and Uday Maitra

Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560012, Karnataka, India, E-mail: chatterjee.sayantan025@gmail.com

Table of Contents

POM, AFM and SEM imaging of H-560

POM, AFM and SEM imaging were carried out on Olympus C3040-ADU, JPK NANO WIZARD II, and FEI Sirion XL30 FEG SEM instruments, respectively. For POM, wet hybrid gel was drop cast on glass slide before experiment. The hybrid material was drop casted on mica sheet and dried under reduced pressure for AFM imaging. AFM measurements were carried out in tapping mode at a scanning rate of 1.0 Hz. For SEM, the dried gel (xerogel) sample was drop casted on silicon wafer and coated with gold of thickness ~10 nm. The operating voltage for FESEM was 20 KeV.

TEM imaging of H-560

TEM images were recorded on JEOL 2100F. For TEM imaging hybrid was drop cast on a carbon-coated copper grid (400 square mesh) and followed by high vacuum drying. Then sample was staining with 0.1% uranyl acetate. The operating voltage for FETEM was 200 KeV.

UV-visible, fluorescence, photoluminescent quantum yield and time resolved spectroscopy of H-560

Absorption and Fluorescence measurements were carried out on a Shimadzu UV-3600 spectrophotometer and Varian Cary Eclipse fluorescence spectrometer. UV-visible absorption and emission spectra of H-560 were recorded on a UV-Vis spectrophotometer and emission at room temperature using quartz cuvette. The photoluminescent quantum yields were recorded on Edinburgh Instruments FLS980 fluorescence spectrometer equipped with an integrating sphere. A light emitting diode (FLSP920) at 405 nm was used as excitation source. Fitting and analysis was performed using Origin8 and Xmgrace software.

Table S1 Gelation behavior of bile acid derived dimeric urea Organogelator **1**

Solvent	Concentration (%w/v)	Remarks[a]	**CGC (%w/v)**
O-xylene	1.0	WG	-
1,2-DCB	1.0	G	0.6
1,3-DCB	1.0	G	0.7
$CHCl_3$	1.0	G	0.9

[a]WG= weak gel; G= Gel; CGC= critical gelation concentration

Thermal stability of the organogel 1

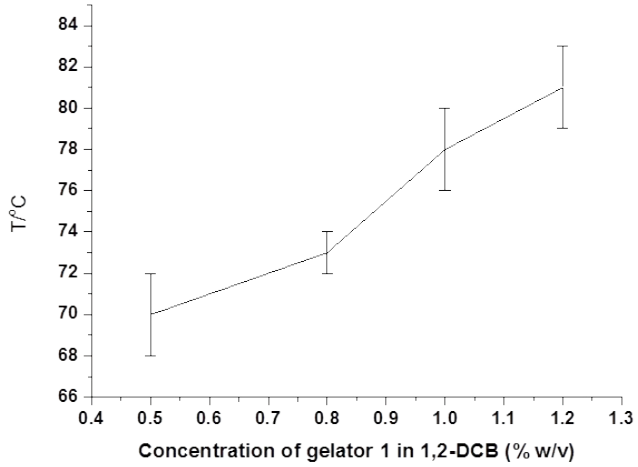

Fig. S1 Gel melting temperatures of the organogel **1** prepared in 1,2-DCB.

Table S2 Computational data for Compound **1**

Energy: -2174.39112865 a.u.

Coordinates:

		Coordinates		
Entry	**Atom**	**x**	**y**	**z**
1	C	10.6188	-1.3761	0.7283
2	C	9.4408	-0.8409	1.5465
3	C	8.5736	0.3765	-0.4987
4	C	12.5195	1.4259	-1.2343
5	C	11.7994	0.7867	-0.026
6	C	11.0126	-0.4684	-0.4522
7	C	9.7991	-0.0752	-1.3693
8	C	10.2281	1.1269	-2.2795
9	C	11.7376	1.1832	2.5359
10	C	7.335	0.7576	-1.346
11	C	8.2116	-0.6005	0.657
12	C	7.0359	-0.0091	1.4474
13	C	5.7634	0.2598	0.5992
14	C	6.1443	1.2624	-0.5051
15	C	6.5064	-0.7325	2.7001
16	C	5.095	-0.1089	2.9333
17	C	4.8272	0.825	1.7113
18	C	3.3414	1.1266	1.3589
19	C	2.8513	2.3446	2.1675
20	C	5.1897	-1.0277	-0.0317
21	C	9.4609	-1.2837	-2.2689
22	O	12.6442	2.8444	-1.0796
23	C	2.3701	-0.0638	1.5341

24	C	1.0591	0.0969	0.7574
25	N	-1.7806	-2.23	0.6314
26	C	-2.8413	-2.7221	-0.2451
27	C	-3.8567	-3.5274	0.5719
28	C	-5.0578	-4.1061	-0.2124
29	C	-4.5721	-5.114	-1.2751
30	C	-7.2172	-3.7468	-1.5695
31	C	-8.4183	-2.7655	-1.4926
32	C	-6.0126	-3.0603	-0.8413
33	C	-7.8087	-1.4831	-0.9061
34	C	-6.7046	-1.9875	0.0693
35	C	-5.8602	-0.7543	0.4533
36	C	-8.7425	-0.41	-0.3288
37	C	-7.8926	0.8089	0.1206
38	C	-10.6935	1.1377	-0.7646
39	C	-9.8036	0.0372	-1.3465
40	C	-6.7271	0.3799	1.0406
41	C	-9.9104	2.3695	-0.2728
42	C	-8.7281	2.0078	0.6965
43	C	-7.7842	3.2527	0.8217
44	C	-8.5017	4.583	0.5694
45	C	-9.0221	4.6743	-0.8748
46	C	-9.4131	3.2799	-1.4128
47	O	-7.9792	5.2653	-1.6582
48	C	-9.3216	1.6901	2.0865
49	C	-7.2912	-2.6559	1.3325
50	N	0.1841	-1.0483	0.997
51	C	-0.904	-1.2618	0.1615
52	O	-1.0748	-0.6544	-0.8892
53	H	11.4958	-1.5265	1.3725
54	H	10.3529	-2.3707	0.3446
55	H	9.1962	-1.5489	2.3485
56	H	9.7187	0.1023	2.0411
57	H	8.8934	1.3048	0.0037
58	H	13.5236	0.9816	-1.3352
59	H	12.5246	0.5348	0.7601
60	H	11.1233	1.5398	0.3975
61	H	11.7002	-1.0629	-1.0721
62	H	9.6882	1.083	-3.2329
63	H	9.9368	2.0736	-1.8069
64	H	11.984	1.9898	-3.2349
65	H	12.081	0.2496	-2.9988
66	H	7.0111	-0.1032	-1.9415
67	H	7.6102	1.5347	-2.0684
68	H	7.9092	-1.5714	0.2359
69	H	7.3759	0.9843	1.7877
70	H	5.2928	1.4677	-1.1689
71	H	6.4134	2.2207	-0.0363
72	H	7.1647	-0.6004	3.5648
73	H	6.4311	-1.8132	2.5252
74	H	5.0504	0.4516	3.8735
75	H	4.34	-0.8973	3.009
76	H	5.2679	1.8008	1.9633
77	H	3.3194	1.4134	0.2962
78	H	1.8112	2.6005	1.9385
79	H	3.462	3.2296	1.9551
80	H	2.9149	2.1482	3.2458
81	H	4.2881	-0.8032	-0.6131
82	H	5.8986	-1.5035	-0.7148
83	H	4.9199	-1.7759	0.7204

84	H	10.3278	-1.5521	-2.8853
85	H	9.1858	-2.1724	-1.6903
86	H	8.6351	-1.0641	-2.9529
87	H	13.0521	3.0085	-0.2146
88	H	2.1436	-0.1857	2.6046
89	H	2.8325	-1.0007	1.2103
90	H	1.2495	0.1339	-0.3186
91	H	0.5542	1.039	1.0177
92	H	-1.3766	-2.9266	1.2468
93	H	-3.3011	-1.8469	-0.7083
94	H	-2.4272	-3.3306	-1.0622
95	H	-3.3317	-4.3761	1.039
96	H	-4.2091	-2.9018	1.3985
97	H	-5.6433	-4.68	0.5207
98	H	-5.3999	-5.7011	-1.684
99	H	-3.852	-5.819	-0.8415
100	H	-4.0796	-4.6122	-2.1166
101	H	-6.9604	-3.9884	-2.6057
102	H	-7.4635	-4.699	-1.0839
103	H	-9.2075	-3.1579	-0.839
104	H	-8.8779	-2.5976	-2.4719
105	H	-5.443	-2.5008	-1.5988
106	H	-7.2623	-0.9951	-1.7317
107	H	-5.0768	-1.0041	1.1781
108	H	-5.3457	-0.3836	-0.445
109	H	-9.272	-0.8268	0.5414
110	H	-7.4257	1.188	-0.8039
111	H	-11.4404	1.458	-1.5039
112	H	-11.2622	0.7162	0.0757
113	H	-9.3018	0.3953	-2.2584
114	H	-10.4239	-0.8154	-1.6505
115	H	-7.1179	0.0606	2.0139
116	H	-6.0802	1.2411	1.2442
117	H	-10.6272	2.9699	0.3072
118	H	-7.3126	3.2635	1.8115
119	H	-6.967	3.1727	0.0938
120	H	-9.3393	4.7026	1.268
121	H	-7.8261	5.4282	0.7407
122	H	-9.9075	5.3315	-0.8926
123	H	-8.5269	2.8456	-1.8922
124	H	-10.1817	3.3742	-2.1924
125	H	-8.2556	5.2284	-2.5875
126	H	-9.8684	2.5596	2.4723
127	H	-10.0254	0.8506	2.0609
128	H	-8.5438	1.4486	2.818
129	H	-6.4899	-2.966	2.013
130	H	-7.9434	-1.9815	1.8942
131	H	-7.8796	-3.5485	1.0942
132	H	0.0369	-1.2761	1.9734

AFM images of the organogelator 1

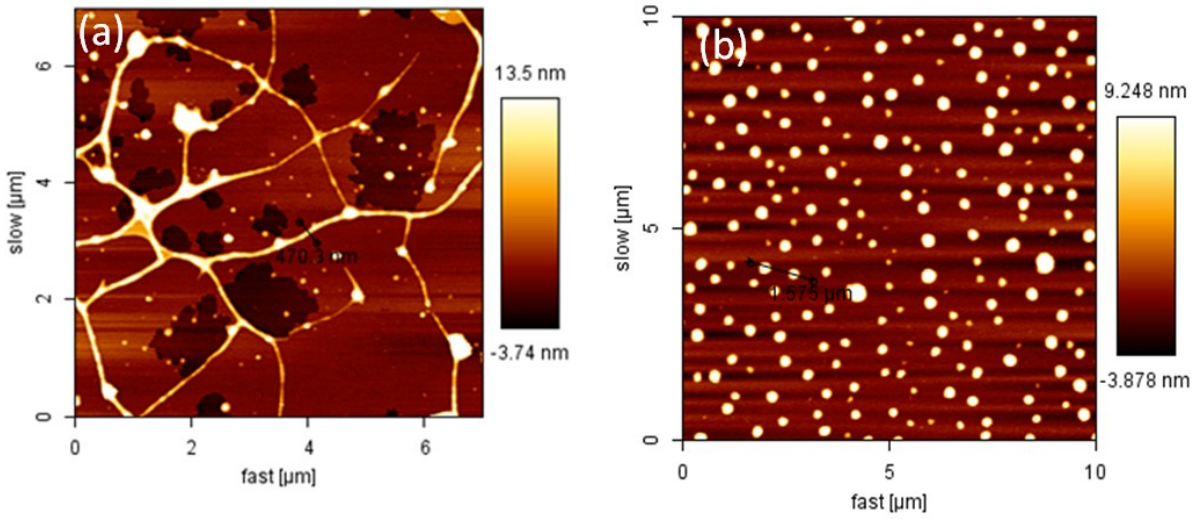

Fig. S2 AFM images of (a) gel in 1,2-DCB (1.0% w/v) and (b) sol (compound **1** in 1,2-DCB) at lower concentration (0.1% w/v).

Fluorescence life-time data fitting

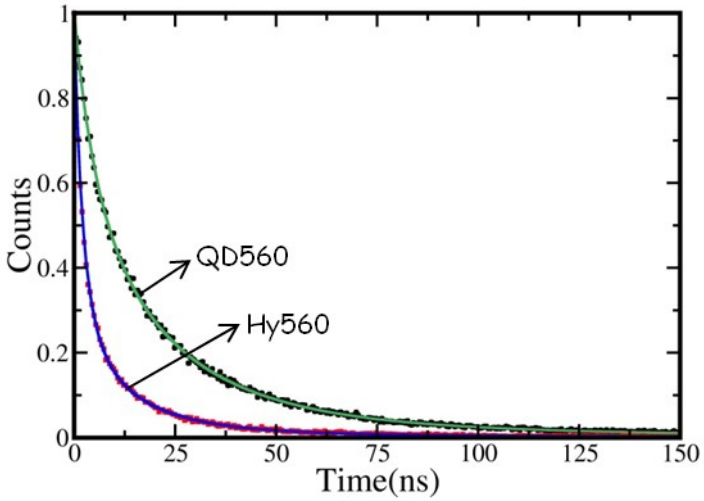

Fig. S3 Fluorescence decay curve fitting using eqn (5).

Temperature dependent steady state fluorescence spectra

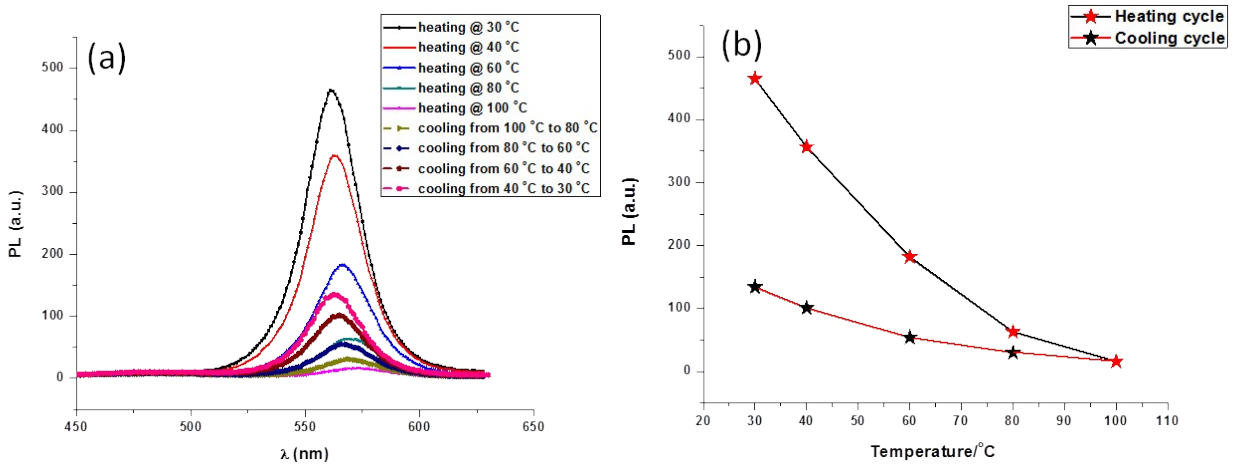

Fig. S4 (a) Temperature-dependent photoluminescence spectra and (b) heating-cooling cycle of green emitting CdSe QDs in 1,2-DCB at different temperatures.

TEM image of nanorod based hybrid gel and QD560

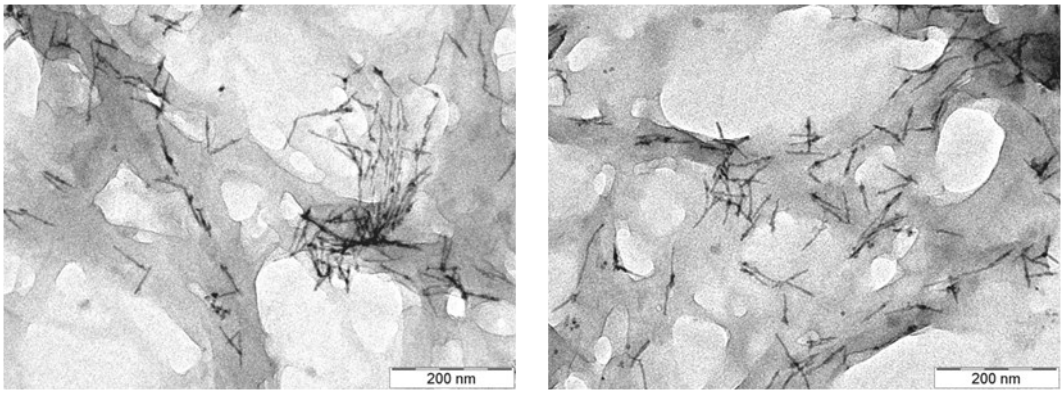

Fig. S5 TEM images of CdSe nanorod-organogel hybrid (scale bar 200 nm).

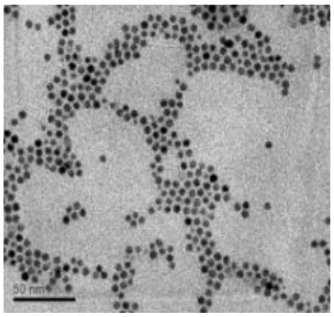

Fig. S6 TEM images of QD560 (scale bar 50 nm).

Copies of NMR spectra: Compound 1:

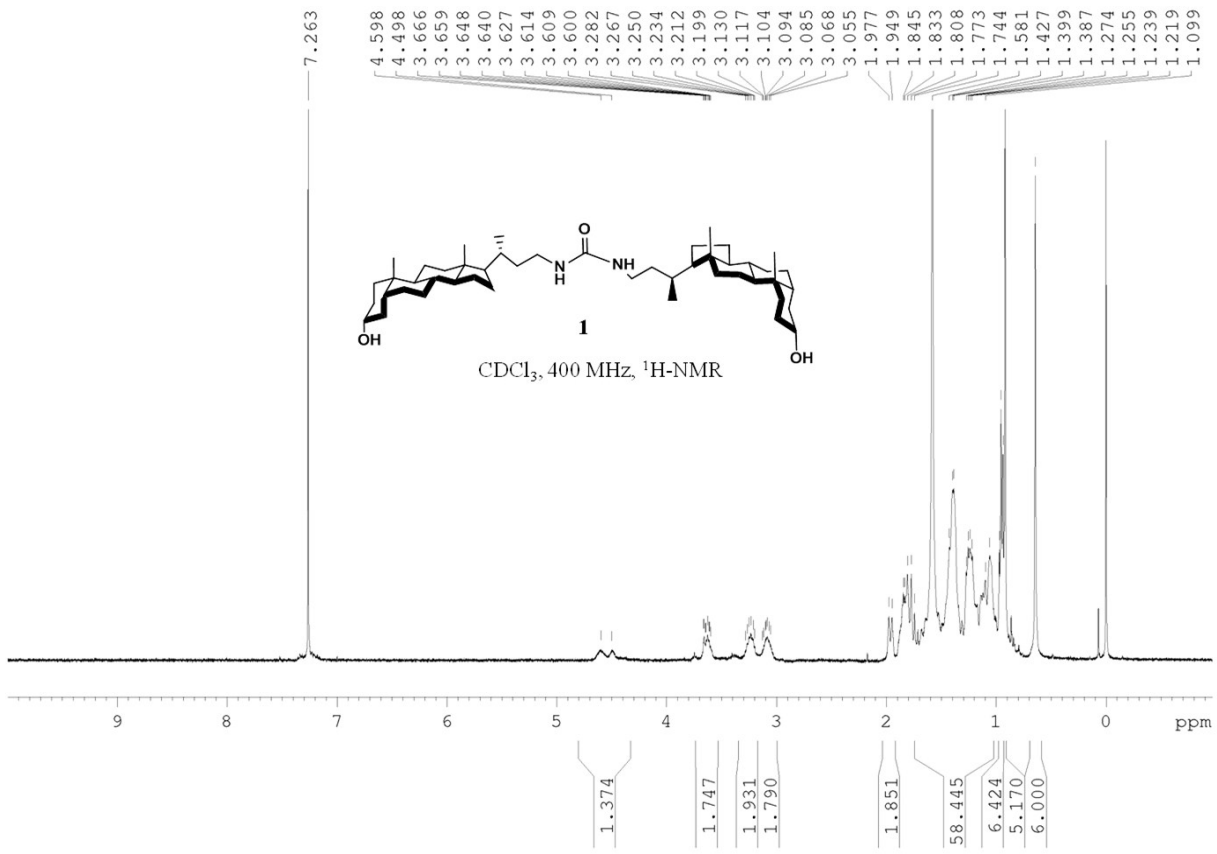

Fig. S7 ^{1}H NMR spectra of Compound **1**.

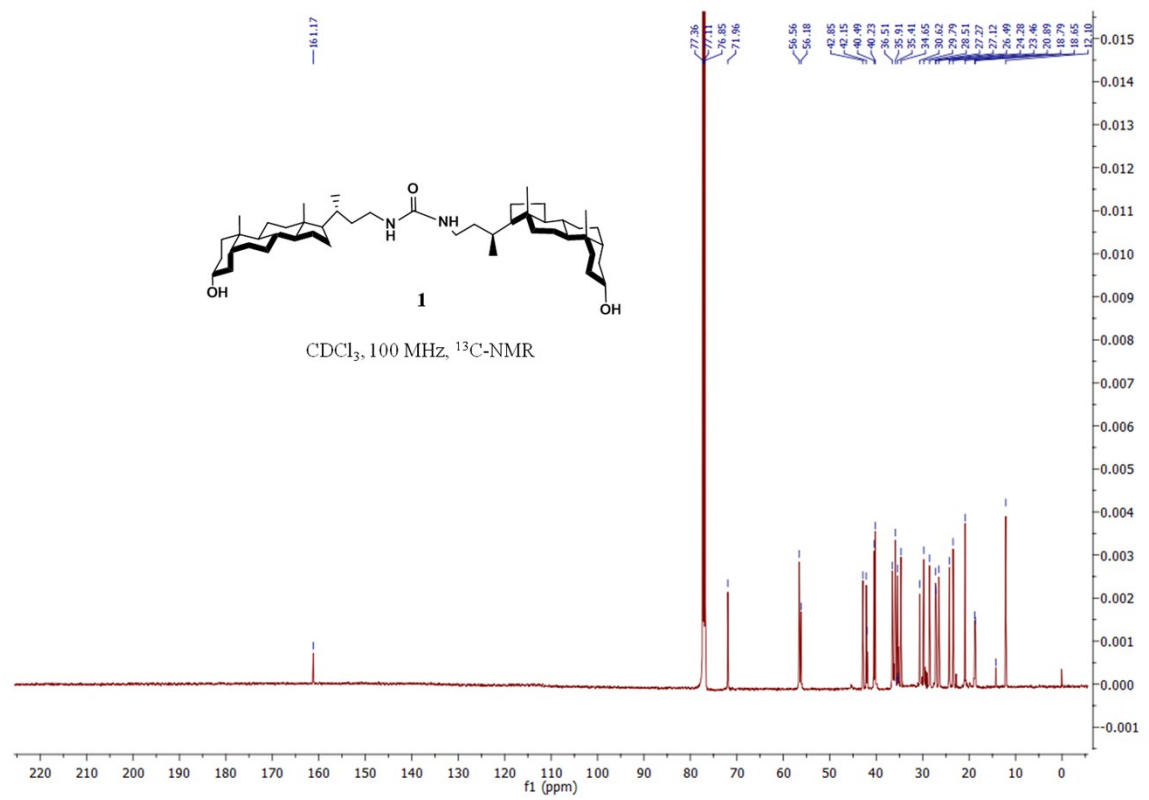

Fig. S8 ^{13}C NMR spectra of Compound **1**.