Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Tuning Properties of Graphene Quantum Dots by Passivation

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Table S1. Absorption energies, wavelengths, and oscillator strengths of $C_{24}H_{12}$ and $C_{24}F_{12}$ GQDs for the first 25 states.

State	Absorption energy (eV)		Wavelength (nm)		Oscillator Strength (f)	
	$C_{24}H_{12}$	$C_{24}F_{12}$	$C_{24}H_{12}$	$C_{24}F_{12}$	$C_{24}H_{12}$	$C_{24}F_{12}$
1	3.27	3.10	378.89	399.52	0.0000	0.0000
2	3.52	3.36	352.06	368.55	0.0000	0.0000
3	4.12	3.94	300.28	314.66	0.9455	0.9462
4	4.13	3.95	300.25	314.64	0.9439	0.9455
5	4.43	4.31	279.80	287.69	0.0000	0.0000
6	4.43	4.31	279.79	287.69	0.0000	0.0000
7	4.46	4.38	277.88	282.78	0.0000	0.0000
8	4.53	4.39	273.51	282.27	0.0000	0.0000
9	4.68	4.46	264.85	277.82	0.0000	0.0000
10	4.77	4.58	259.67	270.87	0.0000	0.0000
11	4.77	4.58	259.66	270.86	0.0000	0.0000
12	5.06	4.72	244.95	262.56	0.0000	0.0000
13	5.06	4.72	244.94	262.54	0.0000	0.0000
14	5.16	4.92	239.88	252.21	0.0000	0.0000
15	5.29	4.96	234.24	249.90	0.0000	0.0000
16	5.29	4.96	234.24	249.88	0.0000	0.0000
17	5.47	5.46	226.50	227.23	0.0000	0.0000
18	5.47	5.46	226.49	227.23	0.0000	0.0000
19	5.63	5.48	220.20	226.05	0.0000	0.0000
20	5.98	5.76	207.18	215.28	0.0000	0.0297
21	6.08	5.76	203.73	215.27	0.0186	0.0295
22	6.08	5.83	203.72	212.79	0.0187	0.0000
23	6.11	5.87	202.88	211.34	0.0000	0.1119
24	6.11	5.87	202.88	211.34	0.0000	0.1117
25	6.21	5.97	199.58	207.70	0.3839	0.0000

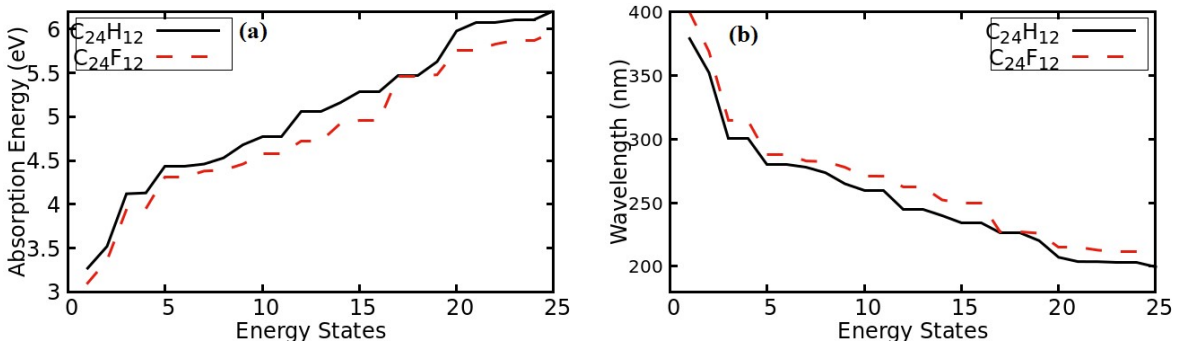

Fig S1. (a) Absorption energy and (b) wavelength of the first 25 energy states of $C_{24}H_{12}$ and $C_{24}F_{12}$ GQDs.

Table S2. Absorption energies, wavelengths, and oscillator strengths of $C_{42}H_{18}$ for the first 25 states.

State	Absorption energy (eV)		Wavelength (nm)		Oscillator Strength (f)	
	$C_{42}H_{18}$	$C_{42}F_{18}$	$C_{42}H_{18}$	$C_{42}F_{18}$	$C_{42}H_{18}$	$C_{42}F_{18}$
1	2.93	2.79	423.01	444.34	0.0000	0.0023
2	3.08	2.93	402.28	422.79	0.0000	0.0184
3	3.36	3.33	368.54	372.88	0.0000	0.9380
4	3.37	3.33	368.40	372.18	0.0000	0.9340
5	3.46	3.37	358.12	367.59	1.0609	0.1181
6	3.46	3.42	358.10	362.75	1.0612	0.0832
7	3.64	3.61	340.31	343.36	0.0001	0.0013
8	3.64	3.66	340.19	338.38	0.0003	0.0374
9	3.89	4.00	318.52	309.75	0.0000	0.0018
10	4.08	4.01	304.13	309.30	0.0000	0.0014
11	4.08	4.06	304.04	305.06	0.0000	0.0027
12	4.25	4.10	291.77	302.67	0.0004	0.0017
13	4.25	4.15	291.75	299.03	0.0004	0.0005
14	4.32	4.19	287.18	296.03	0.0000	0.0003
15	4.39	4.19	282.45	295.91	0.0000	0.0080
16	4.40	4.20	281.68	295.23	0.0000	0.0000
17	4.44	4.22	278.98	294.07	0.0009	0.0063
18	4.45	4.27	278.87	290.58	0.0009	0.0114
19	4.48	4.28	276.53	289.93	0.0000	0.0082
20	4.48	4.29	276.50	288.91	0.0000	0.0014
21	4.54	4.31	272.90	288.00	0.0000	0.0037
22	4.57	4.34	271.33	285.76	0.0000	0.0000
23	4.63	4.34	267.77	285.54	0.0000	0.0142
24	4.63	4.39	267.73	282.64	0.0000	0.0005
25	4.67	4.41	265.73	280.85	0.0000	0.0004

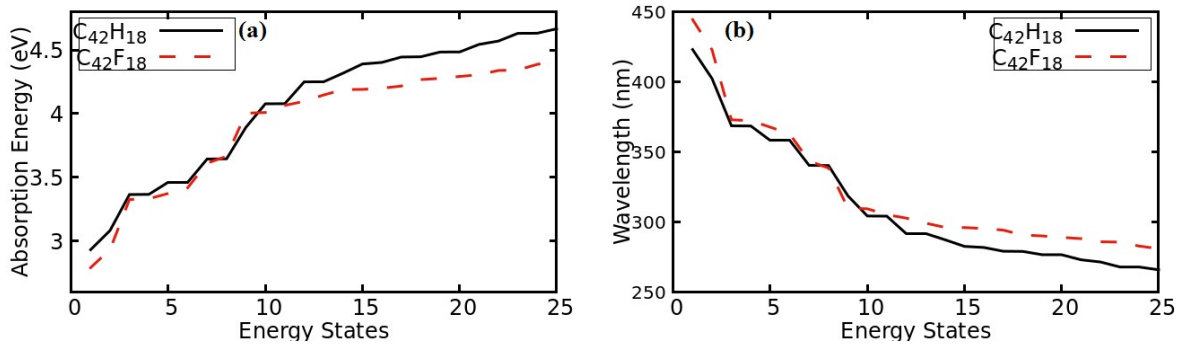

Fig S2. (a) Absorption energy and (b) wavelength of the first 25 energy states of $C_{42}H_{18}$ and $C_{42}F_{18}$ GQDs.

Table S3. Absorption energies, wavelengths, and oscillator strengths of $C_{54}H_{18}$ and $C_{54}F_{18}$ GQDs for the first 25 states.

State	Absorption energy (eV)		Wavelength (nm)		Oscillator Strength (f)	
	$C_{54}H_{18}$	$C_{54}F_{18}$	$C_{54}H_{18}$	$C_{54}F_{18}$	$C_{54}H_{18}$	$C_{54}F_{18}$
1	2.27	2.16	546.57	574.48	0.0000	0.0000
2	2.43	2.33	509.38	532.00	0.0000	0.0000
3	2.87	2.74	432.28	452.05	1.3887	1.3548
4	2.87	2.74	432.27	452.04	1.3877	1.3542
5	3.17	3.05	391.45	406.04	0.0000	0.0000
6	3.17	3.05	391.44	406.04	0.0000	0.0000
7	3.19	3.08	389.19	401.95	0.0000	0.0000
8	3.26	3.14	380.62	394.57	0.0000	0.0000
9	3.30	3.16	375.99	392.88	0.0000	0.0000
10	3.36	3.21	369.41	386.04	0.0000	0.0000
11	3.36	3.21	369.40	386.02	0.0000	0.0000
12	3.53	3.27	350.84	378.83	0.0000	0.0000
13	3.53	3.27	350.80	378.82	0.0000	0.0000
14	3.67	3.50	337.57	353.73	0.0000	0.0000
15	3.74	3.61	331.74	343.66	0.0000	0.0000
16	3.74	3.61	331.73	343.66	0.0000	0.0000
17	3.88	3.86	319.58	321.37	0.0000	0.0000
18	3.90	3.89	317.53	318.72	0.0000	0.0000
19	3.93	3.89	315.82	318.70	0.0314	0.0000
20	3.93	3.91	315.81	317.16	0.0316	0.0039
21	3.96	3.91	312.82	317.15	0.0006	0.0039
22	3.96	3.96	312.81	313.18	0.0005	0.0000
23	4.02	3.97	308.39	312.44	0.0000	0.0000
24	4.02	3.99	308.36	310.61	0.0000	0.0021
25	4.13	3.99	300.16	310.57	0.0000	0.0024

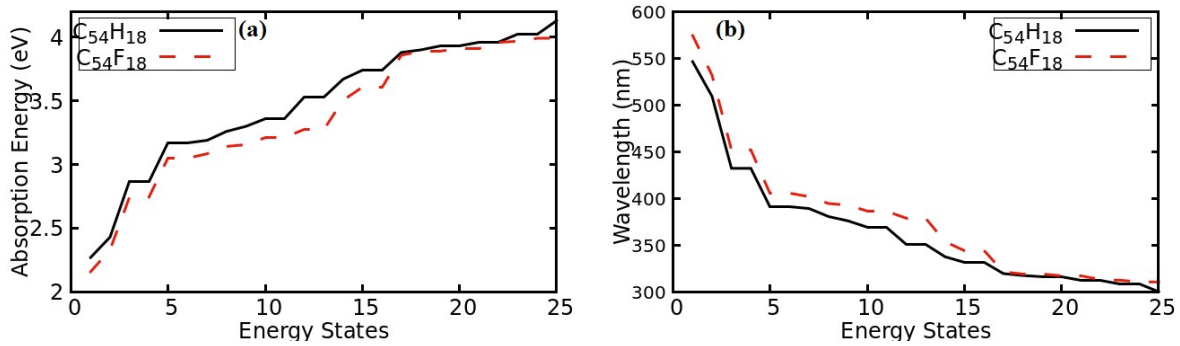

Fig S3. (a)Absorption energy and (b) wavelength of the first 25 energy states $C_{54}H_{18}$ and $C_{54}F_{18}$ GQDs.

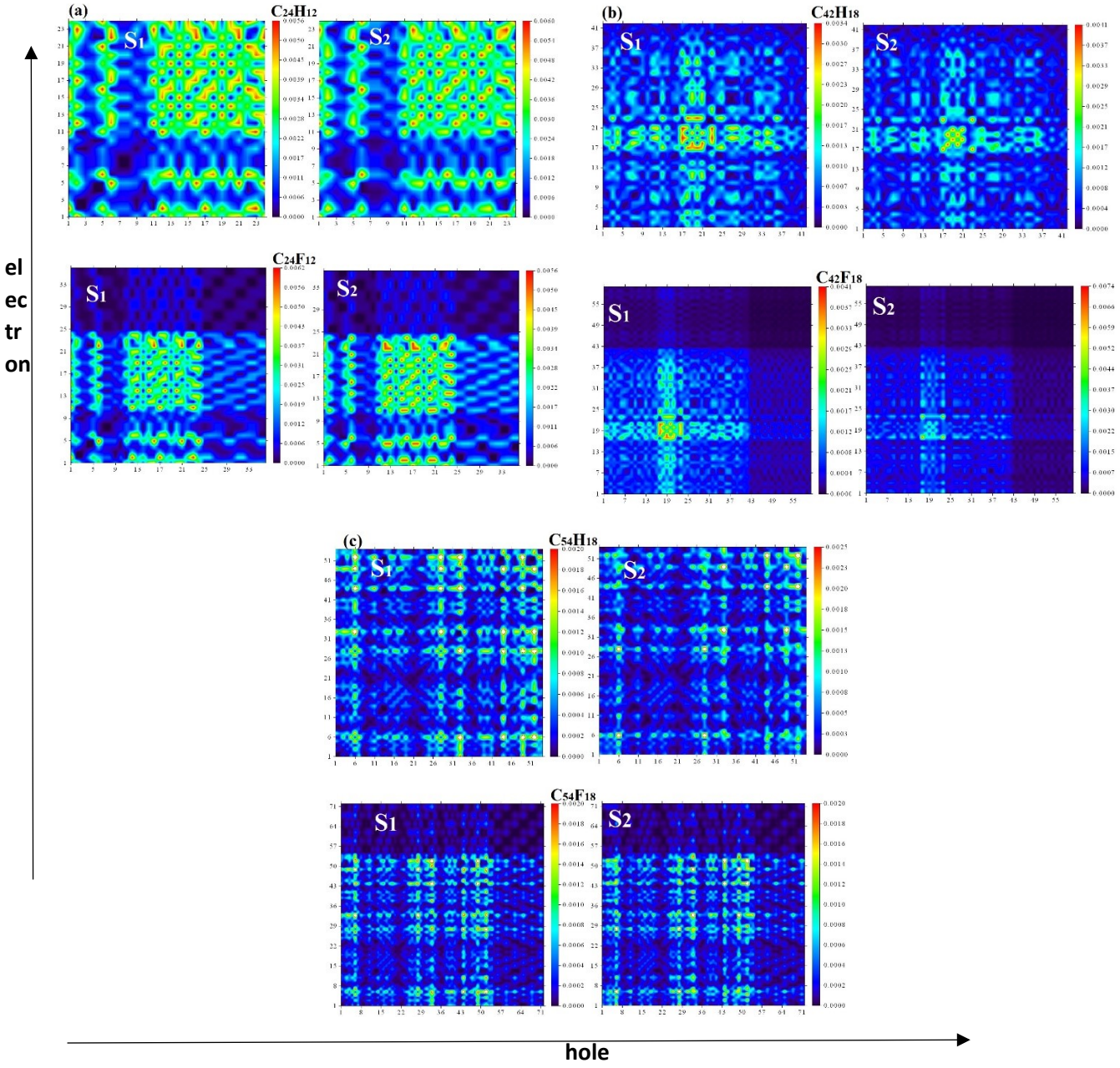

Fig. S4 Color contour of the transition density matrix of S1 and S2 excited states of (a) C24, (b) C42, and (c) C54 GQDs passivated with H and F- atoms respectively. The color bar is shown at the right side of each contour.

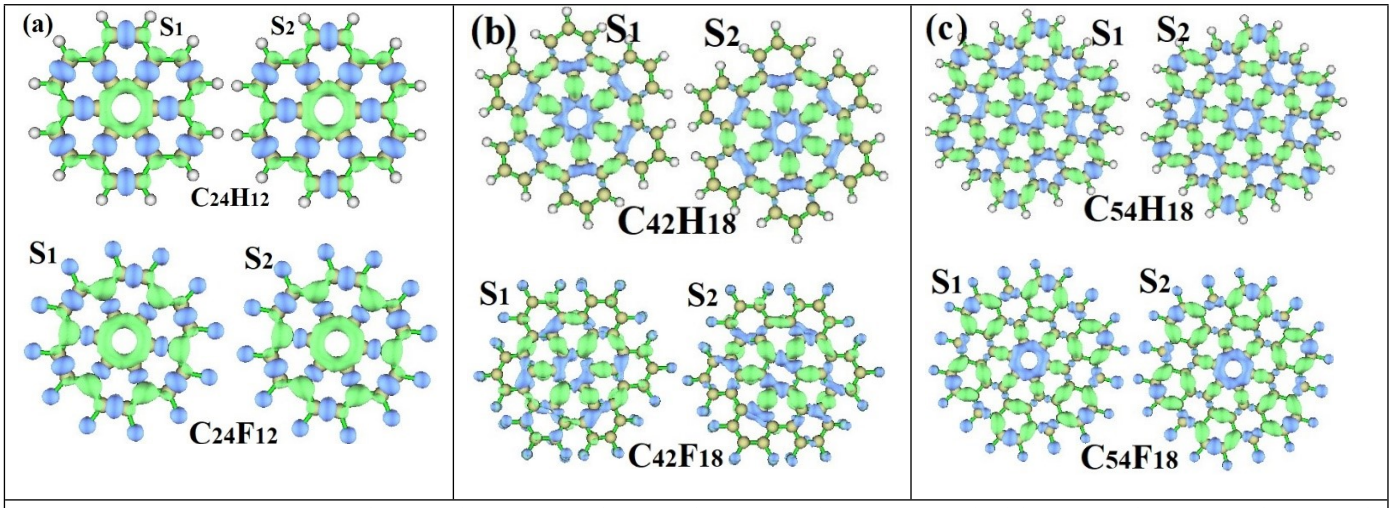

Fig. 7 Representation of charge difference density between the most probable excited state and ground state for (a) C24, (b) C42, and (c) C54 GQDs passivated with h and F-atom. The isosurface value is 0.0004.