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Electronic Supporting Information

Tuning Electronic and Optical Properties of Graphene Quantum Dots by Selective Boronization

Jianguang Feng[a], Hongzhou Dong[a], Beili Pang[a], Yingjie Chen[a], Liyan Yu[*a], and Lifeng Dong[*a,b]

[a] College of Materials Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, China

[b] Department of Physics, Hamline University, St. Paul 55104, USA

[*]Corresponding authors: donglifeng@qust.edu.cn, liyanyu@qust.edu.cn, and ldong03@hamline.edu

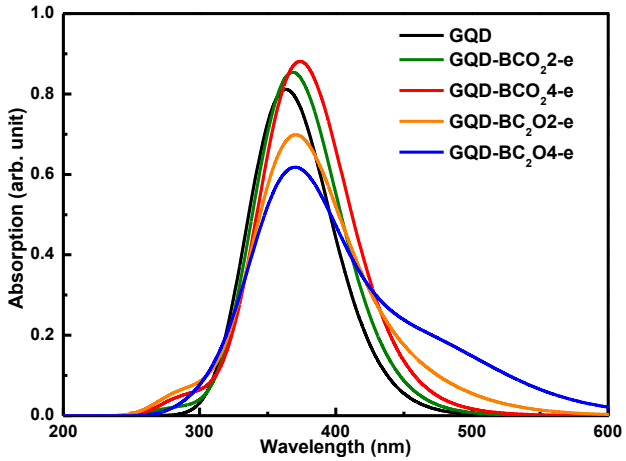

Fig. S1 The calculated absorption spectra of the GQDs with different types and number of oxidized B compounds.

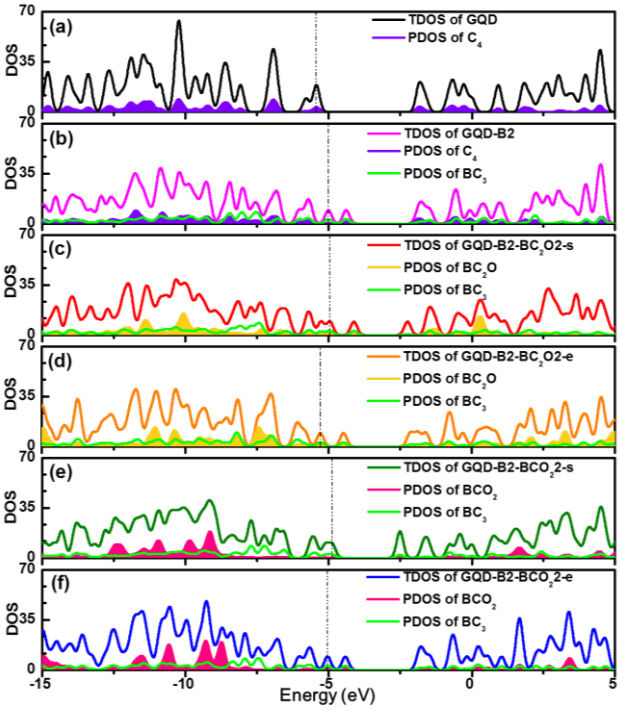

Fig. S2 Density of state (DOS) of pristine GQDs and doped GQDs. (a) pristine GQDs, (b) GQD-B2, (c) GQD-B2-BC_2O2-s, (d) GQD-B2-BC_2O2-e, (e) GQD-B2-$BCO_2$2-s, and (f) GQD-B2-$BCO_2$2, respectively. (The vertical dashed lines indicate the position of the HOMO level. The DOS is plotted with a Gaussian width of 0.01 a.u.).

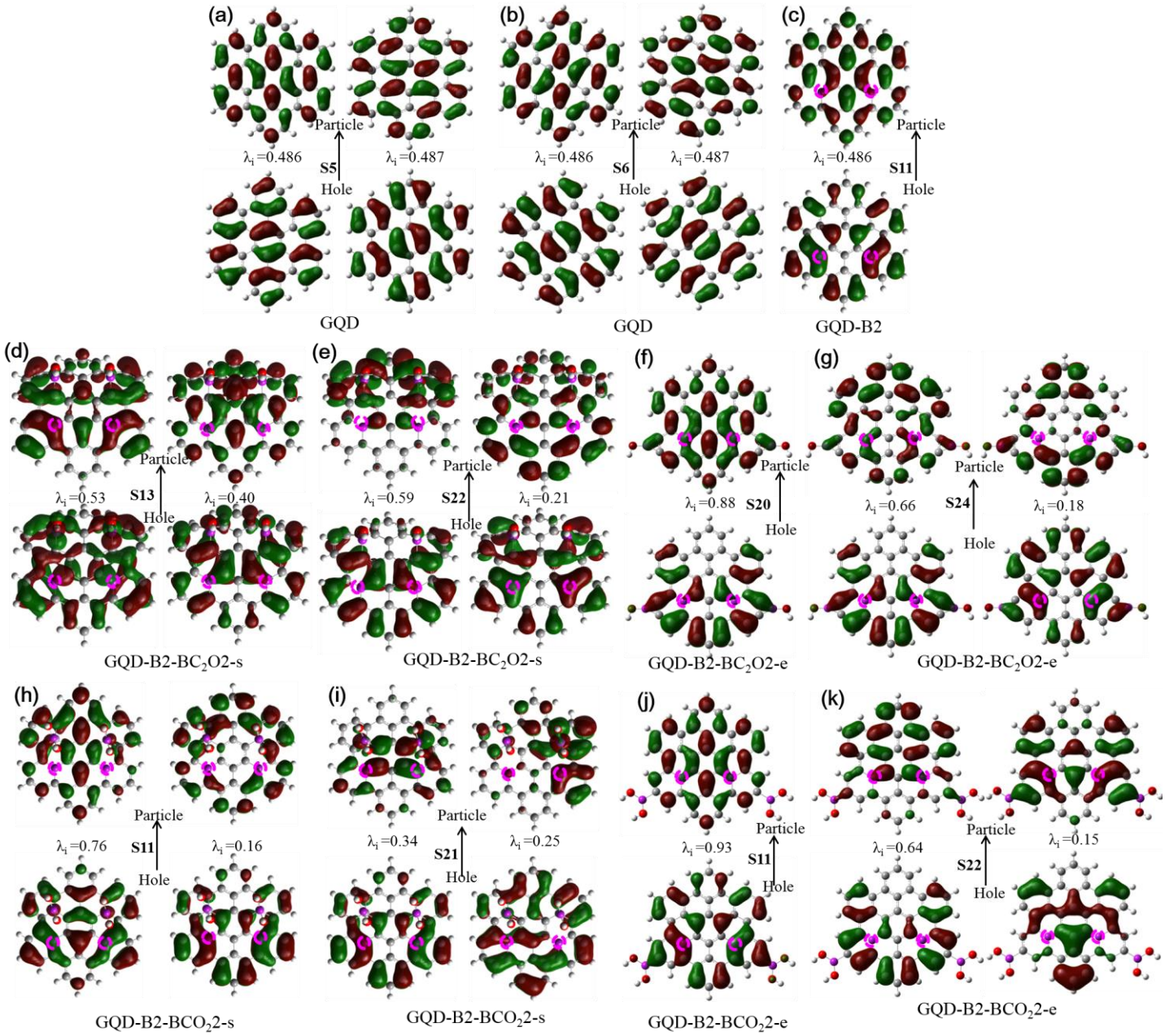

Fig. S3 The NTO pairs for the prominent excited states of doped GQDs. For this state the "hole" is on the left, and the "particle" is on the right; the values represent the associated eigenvalue (λ_i).

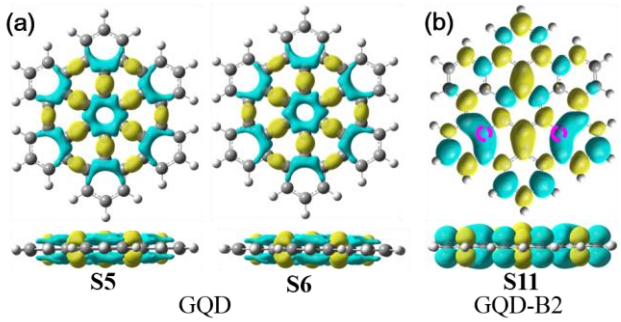

Fig. S4 Representation of the charge difference density between the prominent excited state minus ground state for pristine and B-doped GQDs. Lateral views are displayed at the bottom. (The blue and yellow colors represent holes and electrons, respectively. The isovalue is $4*10^{-4}$).

Table S1 The cartesian coordinates of stationary points for the optimized ground state geometry of pristine GQD and GQD-B2.

Pristine GQD($C_{42}H_{18}$)				GQD-B2($C_{40}B_2H_{18}$)			
	X	Y	Z		X	Y	Z
C	-2.842755	4.928235	-0.00001	**C**	5.689167	0.152664	-0.003542
C	-2.860333	2.497661	-0.000002	**C**	3.565562	1.332765	-0.001306
C	-3.537311	3.726867	-0.000006	**C**	4.967786	1.339056	-0.002758
C	-4.995144	1.20438	0.000006	**C**	3.447822	3.814059	0.000217
C	-2.87248	0.001412	0.000002	**C**	1.361993	2.535466	0.000106
C	-3.591933	1.231772	0.000002	**C**	2.789977	2.576276	-0.000367
C	-4.996326	-1.19947	0.000008	**C**	1.37724	5.01743	0.001462
C	-2.862787	-2.494848	0.000003	**C**	-0.787652	3.827372	0.001347
C	-3.593142	-1.228241	0.000005	**C**	0.638986	3.801724	0.000992
C	-2.847598	-4.925439	0.000004	**C**	-2.964871	4.904226	0.00269
C	-3.540973	-3.723388	0.000005	**C**	-1.587807	5.004302	0.002561
C	1.459587	4.926826	-0.000005	**C**	3.647344	-3.623662	0.001684
C	-1.455133	4.928031	-0.000009	**C**	5.032443	-1.070722	-0.002642
C	-0.728918	3.726704	-0.000006	**C**	3.631903	-1.139612	-0.001035
C	1.43755	2.486983	0	**C**	1.496015	-2.458684	0.000419
C	0.732694	3.726147	-0.000004	**C**	2.924114	-2.422939	0.000323
C	-1.434999	2.488437	-0.000003	**C**	1.448527	0.038899	-0.000195
C	-0.711403	1.233826	-0.000001	**C**	-0.671897	-1.242332	-0.000226
C	1.424431	-0.0007	0.000001	**C**	0.752157	-1.215166	-0.000069
C	0.71288	1.233274	0	**C**	0.685922	1.253774	-0.000066
C	-1.423917	0.0007	0	**C**	-0.737495	1.204516	-0.000112
C	-0.712615	-1.233127	0	**C**	-2.938196	-0.078847	-0.000807
C	1.435104	-2.488395	-0.000002	**C**	-1.434374	-0.038519	-0.000322
C	0.711667	-1.233974	0	**C**	-3.042013	2.442964	0.000159
C	-1.437444	-2.487025	0	**C**	-5.114596	1.061247	-0.002462
C	-0.732581	-3.725986	-0.000002	**C**	-3.711979	1.130739	-0.000949
C	1.454743	-4.928258	-0.000014	**C**	-3.68772	3.661193	0.001529
C	0.729031	-3.726865	-0.000006	**C**	1.644182	-4.936279	0.002326
C	-1.459977	-4.926599	0.000001	**C**	0.841919	-3.761876	0.001227
C	3.54058	3.723962	0.000004	**C**	-0.581173	-3.864054	0.000951
C	2.863012	2.494718	0.000004	**C**	-2.697216	-5.056355	0.00127
C	3.59332	1.228491	0.000006	**C**	-1.31677	-5.082287	0.00155
C	5.689564	-0.002796	0.000012	**C**	-2.906771	-2.602722	-0.000465
C	4.996596	1.199305	0.000011	**C**	-3.48596	-3.854076	0.000344
C	2.872524	-0.001412	0.000003	**C**	-3.646122	-1.328199	-0.00138
C	3.59211	-1.232022	0.000003	**C**	-5.050482	-1.333708	-0.002781
C	4.995415	-1.204215	0.000008	**H**	5.520615	2.269293	-0.0035
C	2.860559	-2.49753	-0.000002	**H**	4.5291	3.856966	0.000061
C	3.536917	-3.727441	-0.000007	**H**	0.84289	5.959781	0.002089
H	-4.619123	3.760836	-0.000006	**H**	-1.15519	6.001584	0.003524
H	-5.564785	2.124754	0.000006	**C**	2.752925	5.027168	0.001105
H	-5.56687	-2.119283	0.000011	**H**	3.301495	5.963904	0.001515
H	-4.622818	-3.756294	0.000007	**C**	-5.783091	-0.154994	-0.00345
C	-5.689425	0.002796	0.000009	**C**	3.018415	-4.872282	0.002681
H	-6.775459	0.00333	0.000012	**H**	6.774712	0.181713	-0.004876
C	2.842247	-4.92863	-0.000014	**H**	5.634448	-1.969941	-0.003427
C	2.847091	4.925834	-0.000001	**H**	4.729338	-3.608605	0.002154
H	-3.38568	5.868839	-0.000013	**H**	3.61632	-5.778339	0.003715
H	-0.943163	5.881537	-0.000012	**H**	1.161024	-5.905942	0.00301
H	0.948606	5.880843	-0.000009	**H**	-0.830979	-6.054768	0.002248
H	3.390482	5.866183	-0.000001	**H**	-3.233972	-6.002173	0.001801
H	4.622261	3.757177	0.000007	**H**	-4.564896	-3.999696	0.000441
H	5.567361	2.118782	0.000013	**H**	-5.581094	-2.279216	-0.003525
H	6.775623	-0.00333	0.000015	**H**	-6.869522	-0.18404	-0.004684
H	5.565276	-2.124252	0.000008	**H**	-5.694953	1.977145	-0.003002
H	4.618565	-3.761719	-0.000007	**H**	-4.772991	3.748173	0.002
H	3.384714	-5.869513	-0.00002	**H**	-3.551677	5.819851	0.003724
H	0.942825	-5.881773	-0.00002	**B**	-1.38949	-2.562328	-0.000032
H	-0.948944	-5.880607	0.000001	**B**	-1.524811	2.484093	0.000289
H	-3.391448	-5.865508	0.000006	**C**	2.884589	0.077391	-0.000767

Table S2 The cartesian coordinates of stationary points for the optimized ground state geometry of GQD–$BCO_2$2-s and GQD–B2–$BCO_2$2-s.

	GQD–$BCO_2$2-s($C_{42}B_2O_4H_{22}$)				GQD–B2–$BCO_2$2-s ($C_{40}B_4O_4H_{22}$)		
	X	Y	Z		X	Y	Z
C	0.022406	5.843414	0.528752	**C**	-0.800182	5.941534	-0.005882
C	-1.218373	3.802193	0.077261	**C**	-1.751305	3.697098	-0.167788
C	-1.185446	5.173808	0.371511	**C**	-1.896214	5.09351	-0.083303
C	-3.695168	3.793745	-0.27442	**C**	-4.245903	3.299586	-0.392565
C	-2.480697	1.678243	-0.259933	**C**	-2.940891	2.841511	-0.25542
C	-2.482178	3.093123	-0.139802	**C**	-5.248134	1.038047	-0.438315
C	-4.893929	1.736514	-0.649747	**C**	-3.750247	-0.975146	-0.323762
C	-3.701841	-0.450318	-0.670916	**C**	-3.967753	0.419395	-0.320985
C	-3.706651	0.988358	-0.533328	**C**	-4.558188	-3.239329	-0.755212
C	-4.727946	-2.550418	-1.364776	**C**	-4.803954	-1.907913	-0.539877
C	-4.739126	-1.153764	-1.259228	**C**	3.226663	4.278366	-0.157739
C	3.722545	3.767301	-0.286346	**C**	0.479457	5.404278	-0.018933
C	1.224882	5.16538	0.366732	**C**	0.703892	4.018027	-0.100741
C	1.246984	3.793495	0.072699	**C**	2.076485	3.497579	-0.127462
C	2.493313	1.660322	-0.264943	**C**	-0.234373	1.650136	-0.193664
C	2.5051	3.075401	-0.147412	**C**	1.248604	-0.315905	-0.215449
C	0.00627	1.652114	-0.180945	**C**	1.069201	1.082594	-0.18624
C	1.21505	-0.476023	-0.190714	**C**	-1.349521	0.768762	-0.187379
C	1.232697	0.933941	-0.206487	**C**	-1.164545	-0.63067	-0.191382
C	-1.225408	0.942433	-0.203315	**C**	0.321928	-2.635565	-0.394692
C	-1.217996	-0.467646	-0.18823	**C**	0.136692	-1.196204	-0.254945
C	-0.009096	-2.655559	-0.147308	**C**	-2.1592	-2.967836	-0.450239
C	-0.003806	-1.184736	-0.186514	**C**	-0.582286	-4.897722	-0.508574
C	-2.488543	-2.666651	-0.403797	**C**	-0.799335	-3.510149	-0.444854
C	-1.217409	-4.775837	-0.094358	**C**	-3.239351	-3.755514	-0.762232
C	-1.235683	-3.371243	-0.190414	**C**	4.775926	2.352278	-0.244444
C	-3.593976	-3.278059	-0.967918	**C**	3.692221	1.426111	-0.229274
C	4.906644	1.701059	-0.658424	**C**	3.831563	0.027542	-0.375942
C	3.714487	0.96125	-0.537541	**C**	5.134875	-1.897437	-1.125415
C	3.700134	-0.47779	-0.669035	**C**	5.062837	-0.579235	-0.754531
C	4.711682	-2.588052	-1.353279	**C**	2.788238	-2.291519	-0.628168
C	4.732863	-1.191306	-1.253641	**C**	3.995536	-2.739152	-1.101014
C	2.471235	-2.684231	-0.392582	**C**	1.629716	-3.179471	-0.534
C	3.572138	-3.305764	-0.953862	**C**	1.795921	-4.573504	-0.595346
C	1.212593	-3.379554	-0.182284	**H**	-2.892052	5.523745	-0.0644
C	1.183971	-4.78418	-0.085089	**H**	-4.477325	4.363013	-0.456349
H	-2.107088	5.727419	0.504988	**H**	-6.164813	0.454297	-0.500831
H	-3.714066	4.874833	-0.210781	**H**	-5.819623	-1.540435	-0.628532
H	-5.836705	1.226572	-0.813984	**C**	-5.360786	2.415733	-0.47264
H	-5.573977	-0.612007	-1.693875	**H**	-6.350374	2.857506	-0.569058
C	-4.886053	3.119277	-0.522187	**C**	4.53371	3.713224	-0.201563
H	-5.814008	3.676979	-0.613542	**H**	-0.942703	7.017038	0.067166
C	4.908323	3.084131	-0.53511	**H**	1.328011	6.07723	0.045638
H	0.026629	6.901013	0.776609	**H**	3.181642	5.367561	-0.157694
H	2.150918	5.712503	0.496651	**H**	5.380433	4.396348	-0.207816
H	3.74902	4.848365	-0.225255	**H**	5.812407	2.019979	-0.272122
H	5.839825	3.635268	-0.630108	**H**	5.941594	0.04623	-0.86177
H	5.845684	1.184329	-0.822865	**H**	6.076966	-2.303687	-1.483501
H	5.571649	-0.65743	-1.690398	**H**	4.099069	-3.748791	-1.47982
H	5.536613	-3.109573	-1.828328	**H**	2.7917	-4.998886	-0.627693
H	3.526793	-4.365087	-1.187827	**H**	-1.421928	-5.580885	-0.47717
H	2.116113	-5.33683	-0.03767	**H**	-3.105215	-4.791126	-1.048311
H	-2.153635	-5.322161	-0.05422	**H**	-5.383677	-3.910847	-0.975035
H	-3.556643	-4.336986	-1.205166	**C**	-0.426526	3.119596	-0.15974
H	-5.556691	-3.063976	-1.841849	**C**	2.653827	-0.891113	-0.108656
C	0.011601	3.090105	-0.031816	**C**	-2.37559	-1.5418	-0.028783
C	2.540611	-1.213414	-0.026234	**B**	2.905346	-1.055347	1.554721
C	-2.548857	-1.197103	-0.030309	**B**	-2.385255	-1.608237	1.659821
B	2.867812	-1.300944	1.588495	**O**	3.593498	-2.151183	1.967586
B	-2.881186	-1.30835	1.581579	**H**	3.74668	-2.187476	2.925419
O	4.180535	-1.392069	1.949464	**O**	2.405421	-0.080184	2.352974
H	4.320387	-1.502244	2.903189	**H**	2.608023	-0.188824	3.295216
O	1.81848	-1.32313	2.457687	**O**	-1.90768	-2.747219	2.228218
H	2.072356	-1.442823	3.386885	**H**	-1.891179	-2.731479	3.198642
O	-1.835057	-1.435578	2.445972	**O**	-2.846324	-0.522014	2.327598
H	-2.095262	-1.563485	3.37229	**H**	-2.772523	-0.57959	3.292722
O	-4.196819	-1.321228	1.943731	**C**	0.700462	-5.426174	-0.567046
H	-4.342545	-1.461539	2.892643	**H**	0.845784	-6.501883	-0.582537
C	-0.019356	-5.476349	-0.00907	**B**	-2.758465	1.336641	-0.22436
H	-0.023571	-6.556296	0.103574	**B**	2.284164	1.995835	-0.153781

Table S3 The cartesian coordinates of stationary points for the optimized ground state geometry of GQD–$BCO_2$2-e and GQD–B2–$BCO_2$2-e.

GQD–$BCO_2$2-e ($C_{42}B_2O_4H_{20}$)				GQD–B2–$BCO_2$2-e ($C_{40}B_4O_4H_{20}$)			
	X	Y	Z		X	Y	Z
C	0.000016	6.244476	-0.000735	**C**	-0.000008	6.249491	-0.06093
C	1.229914	4.14775	0.026474	**C**	-1.237384	4.159297	-0.020611
C	1.201795	5.550965	0.024367	**C**	-1.205692	5.560704	-0.046746
C	3.724732	4.09312	0.093033	**C**	-3.721046	4.108378	0.011163
C	2.48759	1.991099	0.037775	**C**	-2.499238	1.989262	0.00331
C	2.495781	3.416345	0.053328	**C**	-2.501117	3.417306	-0.002453
C	4.926234	2.010358	0.092292	**C**	-4.978915	2.06997	0.026486
C	3.725004	-0.177732	0.019889	**C**	-3.783729	1.299345	0.015776
C	3.725776	1.284784	0.050793	**C**	-5.012773	-2.286827	0.017396
C	4.950057	-2.302594	-0.03362	**C**	-5.040808	-0.897247	0.027858
C	4.922071	-0.906319	0.0003	**C**	3.721017	4.108392	0.011437
C	-3.724751	4.093123	-0.092558	**C**	1.205675	5.560703	-0.046686
C	-1.201772	5.550967	-0.025459	**C**	1.237364	4.159299	-0.020538
C	-1.229908	4.147751	-0.026896	**C**	2.499223	1.989267	0.003417
C	-2.487596	1.9911	-0.037631	**C**	2.501098	3.417313	-0.002301
C	-2.495787	3.416346	-0.053264	**C**	-0.000008	2.009769	-0.004451
C	-0.000002	1.979864	-0.00002	**C**	0.000006	-2.37577	-0.019018
C	-1.232665	-0.156847	-0.008655	**C**	-1.19877	-4.519788	-0.042486
C	-1.23307	1.267551	-0.014229	**C**	-1.232116	-3.116501	-0.02477
C	1.233067	1.267551	0.014219	**C**	-3.761917	-3.021029	-0.004096
C	1.232664	-0.156846	0.008589	**C**	4.978902	2.069991	0.026736
C	0.000002	-2.318402	-0.000224	**C**	3.783721	1.299355	0.01591
C	0	-0.869733	-0.000088	**C**	5.01279	-2.286808	0.017307
C	2.496842	-2.305021	-0.014114	**C**	5.040816	-0.897231	0.027841
C	1.202397	-4.440779	-0.00591	**C**	3.761932	-3.021012	-0.004185
C	1.230627	-3.037699	-0.00795	**C**	1.232132	-3.116494	-0.024777
C	3.726604	-2.976929	-0.039415	**C**	1.198792	-4.519784	-0.042483
C	-4.926255	2.010363	-0.091527	**H**	-2.120401	6.138677	-0.059812
C	-3.725786	1.284785	-0.050381	**H**	-3.735256	5.190382	0.012603
C	-3.725006	-0.177735	-0.019609	**H**	-5.934828	1.560524	0.035668
C	-4.950046	-2.302605	0.033917	**H**	-6.019824	-0.425599	0.044938
C	-4.922068	-0.906327	0.000139	**C**	0.000013	-5.219717	-0.052286
C	-2.496838	-2.305029	0.013861	**C**	4.951769	3.445703	0.025909
C	-3.726592	-2.976941	0.039371	**H**	-0.000007	7.335162	-0.083585
C	-1.230621	-3.037704	0.007306	**H**	2.120388	6.138674	-0.059718
C	-1.20239	-4.440782	0.0047	**H**	3.735218	5.190396	0.012941
H	2.121699	6.121041	0.041182	**H**	5.934818	1.56055	0.035962
H	3.758327	5.17478	0.110135	**H**	6.019829	-0.425577	0.044905
H	5.87907	1.497438	0.111271	**H**	3.866286	-4.104157	-0.01192
H	5.87256	-0.388343	0.004501	**H**	2.129613	-5.075857	-0.048794
C	4.92561	3.398055	0.114786	**H**	0.000015	-6.306565	-0.066457
H	5.865934	3.940515	0.149	**H**	-2.129589	-5.075866	-0.048808
C	0.000004	-5.133889	-0.000759	**H**	-3.866267	-4.104174	-0.011761
C	-4.925636	3.398061	-0.113947	**C**	-0.00001	3.445015	-0.013224
H	0.000023	7.330544	-0.001033	**C**	1.223604	-0.143693	-0.004975
H	-2.121666	6.121048	-0.042613	**C**	-1.223606	-0.143696	-0.005006
H	-3.758356	5.174784	-0.109544	**C**	0.000003	-0.875447	-0.009333
H	-5.86597	3.940524	-0.147823	**B**	-6.366439	-3.085689	0.025785
H	-5.879097	1.497446	-0.110253	**B**	6.366455	-3.085667	0.025607
H	-5.87256	-0.388355	-0.003822	**O**	-7.536359	-2.374542	0.125968
H	-3.752967	-4.058778	0.066177	**H**	-8.337601	-2.919847	0.124711
H	-2.122911	-5.01006	0.005123	**O**	-6.303735	-4.453878	-0.069024
H	0.000006	-6.220033	-0.001002	**H**	-7.165854	-4.8972	-0.064274
H	2.122918	-5.010057	-0.006596	**O**	7.536381	-2.374523	0.125773
H	3.752993	-4.058764	-0.066292	**H**	8.337622	-2.919828	0.124464
C	0.000001	3.428047	-0.000126	**O**	6.303752	-4.453853	-0.069251
C	-2.48576	-0.880434	-0.006974	**H**	7.165873	-4.897171	-0.064557
C	2.48576	-0.880431	0.006939	**C**	3.844763	-0.127415	0.015449
B	-6.30987	-3.086029	0.066143	**C**	2.527052	-2.410224	-0.010763
B	6.309882	-3.086025	-0.065629	**C**	-2.52704	-2.410237	-0.010749
O	-7.468601	-2.356827	-0.014069	**C**	-3.844764	-0.127427	0.015397
H	-8.279872	-2.886756	0.009997	**C**	-1.235401	1.278903	-0.002416
O	6.2575	-4.452149	-0.173339	**C**	1.235393	1.278906	-0.002375
H	7.123054	-4.888089	-0.19271	**H**	5.873608	4.0189	0.036
O	7.46859	-2.356839	0.014899	**C**	-4.951792	3.445684	0.025581
H	8.279873	-2.886749	-0.00917	**H**	-5.873637	4.018874	0.035569
O	-6.257495	-4.452169	0.173728	**B**	2.523652	-0.896332	-0.000849
H	-7.123059	-4.888086	0.193208	**B**	-2.523647	-0.896341	-0.000885

Table S4 The cartesian coordinates of stationary points for the optimized ground state geometry of GQD–BC_2O2-s and GQD–B2–BC_2O2-s.

GQD–BC_2O2-s($C_{42}B_2O_2H_{20}$)				GQD–B2–BC_2O2-s($C_{40}B_4O_2H_{20}$)			
	X	Y	Z		X	Y	Z
C	5.868723	0.714708	-0.629363	**C**	-0.017181	5.974877	-0.727617
C	3.667768	1.691609	-0.297494	**C**	-1.245769	3.907031	-0.325934
C	5.046817	1.829302	-0.518151	**C**	-1.215554	5.287003	-0.588302
C	3.299767	4.163557	-0.232091	**C**	-3.775796	3.808886	-0.216271
C	1.397767	2.670821	0.097657	**C**	-2.533084	3.210102	-0.142526
C	2.792055	2.857484	-0.144902	**C**	-5.056292	1.719336	0.241232
C	1.113366	5.10436	0.133384	**C**	-3.754009	-0.43227	0.564651
C	-0.862949	3.615814	0.510324	**C**	-3.852543	0.966738	0.359166
C	0.555376	3.82118	0.245471	**C**	-4.902374	-2.564681	-0.147799
C	-3.121753	4.540599	-0.106028	**C**	-4.901025	-1.319098	0.446046
C	-1.830404	4.666754	0.41256	**C**	3.753801	3.830678	-0.215519
C	4.206076	-3.248863	-0.209329	**C**	1.185138	5.293895	-0.588214
C	5.339737	-0.56427	-0.508656	**C**	1.223269	3.914154	-0.325792
C	3.967757	-0.761584	-0.289085	**C**	2.514559	3.224652	-0.142296
C	1.998693	-2.256812	0.105535	**C**	-0.004927	1.702381	-0.009813
C	3.3982	-2.103257	-0.131098	**C**	1.209649	-0.436739	0.338239
C	1.700061	0.206947	-0.0113	**C**	1.204195	0.98359	0.145103
C	-0.268246	-1.245896	0.310955	**C**	-1.209801	0.976703	0.144874
C	1.140875	-1.087835	0.128909	**C**	-1.207096	-0.443577	0.338136
C	0.846452	1.329859	0.126199	**C**	0.007636	-2.654812	-0.38896
C	-0.558932	1.145271	0.310592	**C**	0.003678	-1.248695	0.185307
C	-2.627153	-0.318879	-0.379351	**C**	-2.492365	-3.115469	-0.157174
C	-1.20398	-0.14644	0.151138	**C**	-1.177599	-4.313596	-1.827577
C	-3.412157	2.096775	-0.112782	**C**	-1.210645	-3.340867	-0.818164
C	-4.466687	0.656109	-1.76819	**C**	-3.757932	-3.244761	-0.694221
C	-3.480038	0.804249	-0.779243	**C**	5.046195	1.74819	0.241252
C	-3.737141	3.355888	-0.598393	**C**	3.846957	0.988639	0.358828
C	2.308561	-4.687167	0.149871	**C**	3.756541	-0.411113	0.564201
C	1.457145	-3.57584	0.252567	**C**	4.917013	-2.536965	-0.148203
C	0.029047	-3.717442	0.506439	**C**	4.908579	-1.291131	0.44532
C	-1.935405	-5.155881	-0.134048	**C**	2.510091	-3.101246	-0.157076
C	-0.656718	-4.969894	0.397367	**C**	3.776546	-3.223849	-0.693939
C	-2.805971	-2.854702	-0.132693	**C**	1.229802	-3.333919	-0.818151
C	-2.81393	-4.151153	-0.627728	**C**	1.202324	-4.306734	-1.827718
C	-3.182721	-1.61184	-0.790412	**H**	-2.147282	5.834899	-0.67857
C	-4.176754	-1.698518	-1.779075	**H**	-3.897287	4.870409	-0.428011
H	5.498554	2.80998	-0.599752	**H**	-6.034848	1.25899	0.361832
H	4.353137	4.331798	-0.417791	**H**	-5.877056	-0.894349	0.665555
H	0.483821	5.981336	0.229373	**C**	-4.99582	3.073226	-0.021557
H	-1.485901	5.689832	0.530399	**H**	-5.927123	3.630624	-0.09421
C	2.472495	5.272322	-0.09357	**C**	4.977876	3.101924	-0.020951
H	2.891649	6.27165	-0.167823	**H**	-0.02024	7.042606	-0.931329
C	3.669562	-4.523726	-0.068642	**H**	2.113707	5.847114	-0.67849
H	6.933508	0.844352	-0.800266	**H**	3.869221	4.89297	-0.426747
H	6.014736	-1.407632	-0.582335	**H**	5.906	3.664649	-0.093267
H	5.26991	-3.159256	-0.390035	**H**	6.027444	1.293545	0.361617
H	4.317482	-5.392974	-0.135264	**H**	5.88222	-0.860533	0.664026
H	1.908362	-5.689634	0.247188	**H**	5.895451	-2.956179	-0.376494
H	-0.077464	-5.880647	0.516488	**H**	3.950173	-3.776962	-1.616967
H	-2.186197	-6.186072	-0.382492	**H**	2.13828	-4.758853	-2.137416
H	-3.401305	-4.420831	-1.505613	**H**	-2.110955	-4.771164	-2.137124
H	-4.515833	-2.684094	-2.080539	**H**	-3.928443	-3.797929	-1.617807
H	-5.034511	1.532844	-2.061514	**H**	-5.878397	-2.989755	-0.37561
H	-4.380997	3.480501	-1.469254	**C**	-0.009174	3.184344	-0.218485
H	-3.615884	5.480749	-0.346571	**C**	2.458139	-1.002971	0.737449
C	3.117413	0.379616	-0.205665	**C**	-2.452087	-1.016773	0.737794
C	-0.707049	-2.54079	0.712622	**B**	2.438279	-2.446381	1.226947
C	-1.293361	2.29654	0.71727	**B**	-2.424145	-2.460234	1.226915
B	-2.133074	-2.685761	1.224456	**O**	2.378597	-3.035403	2.437099
B	-2.70804	2.089588	1.238924	**H**	2.345011	-2.388579	3.162288
O	-2.689896	-2.683109	2.453905	**O**	-2.361002	-3.049058	2.43699
H	-2.029152	-2.561498	3.156625	**H**	-2.330881	-2.402148	3.162252
O	-3.237119	1.943895	2.472046	**C**	0.013674	-4.767059	-2.372655
H	-2.56033	1.982633	3.168876	**H**	0.015842	-5.532466	-3.14262
C	-4.786722	-0.575876	-2.314633	**B**	-2.522486	1.719005	0.157942
H	-5.555749	-0.667056	-3.07583	**B**	2.512525	1.733339	0.15785

Table S5 The Cartesian Coordinates of stationary points for the optimized ground state geometry of GQD–BC_2O2-e and GQD–B2–BC_2O2-e.

GQD–BC_2O2-e($C_{42}B_2O_2H_{16}$)				GQD–B2–BC_2O2-e($C_{40}B_4O_2H_{16}$)			
	X	Y	Z		X	Y	Z
C	0.000021	5.871928	0.204008	**C**	0.000002	5.877633	0.250994
C	-1.230181	3.778758	0.085855	**C**	-1.236964	3.794002	0.086321
C	-1.202356	5.179594	0.16167	**C**	-1.20594	5.191018	0.192817
C	-3.73084	3.711291	-0.013548	**C**	-3.71974	3.739034	-0.060802
C	-2.494249	3.047935	0.026535	**C**	-2.497602	3.054811	0.009107
C	-4.923343	1.622291	-0.088635	**C**	-4.978	1.700308	-0.119564
C	-3.706514	-0.526884	-0.06387	**C**	-3.828042	-0.466908	-0.056114
C	-3.709712	0.919989	-0.052117	**C**	-3.772753	0.943902	-0.061055
C	-4.892685	-2.679188	-0.161424	**C**	-4.94973	-2.6629	-0.11674
C	-4.894537	-1.275479	-0.137574	**C**	-5.01489	-1.267757	-0.115796
C	3.730848	3.711276	-0.01398	**C**	3.719741	3.739032	-0.060806
C	1.20239	5.179591	0.161529	**C**	1.205944	5.191017	0.192812
C	1.230201	3.778753	0.085715	**C**	1.236966	3.794001	0.086318
C	2.49426	3.047924	0.026273	**C**	2.497603	3.05481	0.009102
C	0.000005	1.608134	0.03354	**C**	0	1.641999	0.027159
C	1.23241	-0.534509	0.024437	**C**	1.225636	-0.516709	0.033292
C	1.231019	0.894073	0.021447	**C**	1.236214	0.909467	0.021174
C	-1.231015	0.894078	0.021517	**C**	-1.236214	0.909467	0.021178
C	-1.232412	-0.534503	0.024483	**C**	-1.225637	-0.516709	0.033298
C	-0.000004	-2.694535	0.099192	**C**	-0.000001	-2.743065	0.092158
C	-0.000002	-1.24458	0.037183	**C**	0	-1.244995	0.046366
C	-2.503758	-2.700785	0.020603	**C**	-2.536474	-2.800286	0.038203
C	-1.200645	-4.804679	0.330081	**C**	-1.196541	-4.883582	0.257517
C	-1.228414	-3.413205	0.148866	**C**	-1.231152	-3.486485	0.127517
C	-3.707262	-3.408176	-0.085874	**C**	-3.749832	-3.452386	-0.051733
C	4.923337	1.622265	-0.089044	**C**	4.978	1.700306	-0.119572
C	3.709709	0.919967	-0.052348	**C**	3.772753	0.9439	-0.061064
C	3.706514	-0.526912	-0.06393	**C**	3.828041	-0.46691	-0.056123
C	4.892681	-2.679215	-0.161096	**C**	4.949729	-2.662901	-0.11673
C	4.894521	-1.275501	-0.137589	**C**	5.014889	-1.267758	-0.115799
C	2.503747	-2.700802	0.020758	**C**	2.536473	-2.800287	0.038203
C	3.707265	-3.408201	-0.085483	**C**	3.749833	-3.452387	-0.051716
C	1.228397	-3.413216	0.148943	**C**	1.231151	-3.486486	0.127515
C	1.200602	-4.804695	0.330093	**C**	1.196538	-4.883583	0.257512
H	-2.12404	5.746593	0.195953	**H**	-2.122379	5.764318	0.246193
H	-3.77215	4.793257	-0.007425	**H**	-3.73467	4.821286	-0.076285
H	-5.852558	1.065382	-0.131069	**H**	-5.91617	1.157216	-0.16267
C	-4.931286	3.009224	-0.070803	**C**	-4.952773	3.074225	-0.124964
C	4.931285	3.009201	-0.071319	**C**	4.952774	3.074223	-0.124969
H	0.000026	6.955977	0.269017	**H**	0.000003	6.959482	0.343611
H	2.124079	5.746587	0.195707	**H**	2.122384	5.764316	0.246183
H	3.772162	4.793242	-0.007928	**H**	3.734672	4.821284	-0.076285
H	5.852547	1.065352	-0.131517	**H**	5.916169	1.157213	-0.162679
H	3.716147	-4.490928	-0.120635	**H**	3.839773	-4.53665	-0.082914
H	2.122068	-5.364898	0.420256	**H**	2.126513	-5.436933	0.315288
H	-2.122125	-5.36485	0.420299	**H**	-2.126517	-5.43693	0.315299
H	-3.716109	-4.490891	-0.121379	**H**	-3.839771	-4.536648	-0.082948
C	0.000007	3.057405	0.063546	**C**	0.000001	3.076923	0.058694
C	2.49112	-1.254617	-0.001314	**C**	-0.000002	-5.58191	0.329372
C	-2.49113	-1.254598	-0.00132	**H**	-0.000002	-6.662803	0.438875
C	-0.000026	-5.492692	0.430591	**B**	6.288663	-2.025883	-0.186166
H	-0.00003	-6.56664	0.590218	**B**	-6.288663	-2.025882	-0.186174
B	6.198651	-1.974342	-0.23786	**C**	2.490353	1.628666	-0.006736
B	-6.19864	-1.974322	-0.2383	**C**	-2.490353	1.628667	-0.00673
C	2.476983	1.624283	0.001869	**O**	7.645222	-2.03078	-0.256269
C	-2.476978	1.624295	0.002056	**H**	8.000906	-2.933038	-0.278245
O	7.54755	-1.910921	-0.32498	**O**	-7.645222	-2.030779	-0.256275
H	7.951624	-2.792006	-0.369907	**H**	-8.000905	-2.933037	-0.278263
O	-7.547543	-1.910938	-0.325346	**H**	5.871439	3.650023	-0.177805
H	-7.951579	-2.792042	-0.370249	**H**	-5.871438	3.650026	-0.177801
H	5.871958	3.551164	-0.102863	**B**	-2.53151	-1.265827	0.015484
H	-5.87196	3.551194	-0.102209	**B**	2.531509	-1.265828	0.015475

Table S6 The excitation energies, wavelengths, oscillator strengths, transition coefficients, and associated eigenvalues of the dominated excitation in GQDs.

GQDs	Dominant Excitation	Excitation energy(eV)	Wavelength (nm)	Oscillator strength (f)	Transition coefficients	λ_i
GQD	S5	3.41	363.51	1.00	H→L -0.45	0.49
					H-1→L+1 0.45	0.49
	S6	3.41	363.50	1.00	H-1→L 0.45	0.49
					H→L+1 0.45	0.49
GQD-B2	S11	2.71	457.48	0.36	H→L+1 0.68	0.93
GQD-B2-BC_2O2-s	S13	2.6679	464.73	0.32	H-8→L9 0.48	0.53
					H-1→L+1 0.41	0.40
	S22	3.3182	373.65	0.62	H-2→L+1 0.19	0.59
					H-1→L+2 0.52	0.21
					H→L+3 -0.34	
GQD-B2-BC_2O2-e	S20	3.2395	382.73	0.30	H-1→L+1 0.66	0.88
	S24	3.579	346.42	0.38	H-13 →L -0.19	0.66
					H-1→L+2 0.57	0.18
					H→L+3 0.23	
					H→L+4 0.19	
GQD-B2-$BCO_2$2-s	S11	3.0185	410.74	0.25	H-1→L+2 0.61	0.76
					H→L+3 0.28	0.16
	S21	3.6948	335.57	0.38	H-7→L+1 0.22	0.34
					H-5→L 0.26	0.25
					H-3→L+3 0.28	
					H→L+4 0.41	
GQD-B2-$BCO_2$2-e	S11	2.7418	452.2	0.39	H→L+1 0.68	0.93
	S22	3.5224	351.99	0.36	H-15→L 0.21	0.64
					H-1→L+2 0.53	0.15
					H-1→L+3 0.19	
					H→L+3 -0.27	

Table S7 Absorption energies, wavelengths, and oscillator strengths for the first 25 singlet states. The values were obtained using B3LYP/6-31G* for the optimized ground state geometry. Water was considered as solvent by using the polarizable continuum model.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
Pristine GQD	1	2.90	428.24	0.0000
	2	3.03	409.46	0.0000
	3	3.31	374.98	0.0000
	4	3.31	374.96	0.0000
	5	3.41	363.51	1.0023
	6	3.41	363.50	1.0018
	7	3.58	346.24	0.0000
	8	3.58	346.23	0.0000
	9	3.82	324.80	0.0000
	10	3.97	312.32	0.0000
	11	3.97	312.31	0.0000
	12	4.16	298.25	0.0002
	13	4.16	298.24	0.0002
	14	4.23	293.26	0.0000
	15	4.29	289.22	0.0000
	16	4.31	287.52	0.0000
	17	4.37	283.69	0.0008
	18	4.37	283.68	0.0008
	19	4.42	280.38	0.0000
	20	4.42	280.38	0.0000
	21	4.47	277.66	0.0000
	22	4.51	275.15	0.0000
	23	4.55	272.35	0.0000
	24	4.55	272.35	0.0000
	25	4.58	270.81	0.0000

Table S8 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of C42-B2.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
	1	0.1014	12222.99	0.0009
	2	0.8069	1536.51	0.0070
	3	0.9953	1245.71	0.0488
	4	1.17	1063.32	0.2017
	5	1.90	653.57	0.0159
	6	1.98	627.20	0.0210
	7	2.12	585.80	0.1311
	8	2.20	564.00	0.0298
	9	2.28	544.57	0.0000
C42-B2	10	2.48	499.11	0.0000
	11	2.71	457.48	0.3605
	12	2.88	431.25	0.0238
	13	2.90	428.14	0.0000
	14	3.00	413.95	0.0034
	15	3.09	401.04	0.1246
	16	3.18	389.58	0.0265
	17	3.30	375.95	0.0001
	18	3.33	372.22	0.0695
	19	3.41	363.90	0.2014
	20	3.46	358.18	0.0170
	21	3.50	354.06	0.0027
	22	3.58	346.07	0.2261
	23	3.60	344.40	0.1944
	24	3.62	342.63	0.0018
	25	3.75	330.49.	0.1881

Table S9 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of C42-BC_2O2-s.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths (f)
C42-BC_2O2-s	1	2.4958	496.78	0.1267
	2	2.6109	474.87	0.1464
	3	2.9237	424.07	0.0053
	4	3.0671	404.24	0.3532
	5	3.1253	396.71	0.6160
	6	3.2337	383.41	0.1982
	7	3.2769	378.35	0.1202
	8	3.3097	374.61	0.0053
	9	3.3393	371.29	0.0174
	10	3.4397	360.45	0.0075
	11	3.5134	352.89	0.0016
	12	3.5291	351.32	0.0847
	13	3.6582	338.92	0.0064
	14	3.7482	330.78	0.0342
	15	3.7922	326.95	0.0033
	16	3.8538	321.72	0.0079
	17	3.9308	315.41	0.0287
	18	3.9487	313.98	0.0034
	19	4.0071	309.41	0.0135
	20	4.0322	307.48	0.0174
	21	4.0672	304.84	0.0033
	22	4.1025	302.22	0.0271
	23	4.1261	300.48	0.0126
	24	4.1413	299.38	0.0120
	25	4.1888	295.99	0.0002

Table S10 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of C42-BC_2O2-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths (f)
C42-BC_2O2-e	1	2.7804	445.93	0.0575
	2	2.8241	439.02	0.1789
	3	3.0377	408.15	0.0006
	4	3.1694	391.19	0.0005
	5	3.2530	381.14	0.4083
	6	3.3495	370.16	0.5420
	7	3.3898	365.75	0.6736
	8	3.5985	344.54	0.1146
	9	3.688	336.19	0.0096
	10	3.8925	318.52	0.0420
	11	3.9692	312.37	0.0031
	12	4.0035	309.69	0.0003
	13	4.004	309.65	0.0152
	14	4.1315	300.09	0.0067
	15	4.1445	299.16	0.0017
	16	4.1829	296.4	0.0054
	17	4.2267	293.33	0.0270
	18	4.2294	293.15	0.0000
	19	4.2897	289.03	0.0204
	20	4.3295	286.37	0.0021
	21	4.3746	283.42	0.0430
	22	4.3748	283.4	0.0102
	23	4.3809	283.01	0.0008
	24	4.4532	278.42	0.0083
	25	4.4618	277.88	0.0093

Table S11 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of C42-B2-BC_2O2-s.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
C42-B2-BC_2O2-s	1	0.3509	3533.53	0.0034
	2	0.876	1415.27	0.1038
	3	0.9811	1263.73	0.0141
	4	1.1511	1077.14	0.0894
	5	1.789	693.02	0.0336
	6	1.8985	653.06	0.0094
	7	2.0252	612.21	0.0037
	8	2.1622	573.42	0.0519
	9	2.2246	557.33	0.1213
	10	2.5584	484.61	0.1034
	11	2.5837	479.86	0.0317
	12	2.6561	466.79	0.0013
	13	2.6679	464.73	0.3243
	14	2.7902	444.35	0.0127
	15	2.9129	425.64	0.0009
	16	2.9708	417.34	0.0007
	17	3.0064	412.41	0.0019
	18	3.0089	412.05	0.0214
	19	3.0947	400.64	0.0027
	20	3.1293	396.21	0.1826
	21	3.2829	377.67	0.0007
	22	3.3182	373.65	0.6219
	23	3.3709	367.81	0.0046
	24	3.3744	367.43	0.0149
	25	3.4574	358.6	0.0256

Table S12 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of C42-B2-BC_2O2-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
C42-B2-BC_2O2-e	1	0.4201	2951.26	0.0145
	2	1.0136	1223.21	0.0006
	3	1.0564	1173.62	0.0391
	4	1.1637	1065.45	0.2377
	5	1.7563	705.95	0.0000
	6	1.9986	620.36	0.0200
	7	2.0107	616.63	0.0070
	8	2.0367	608.74	0.0002
	9	2.1606	573.85	0.0750
	10	2.2223	557.91	0.1346
	11	2.305	537.89	0.0000
	12	2.3285	532.47	0.0089
	13	2.7012	459.00	0.3221
	14	2.9912	414.50	0.0004
	15	3.0133	411.46	0.0008
	16	3.0383	408.07	0.0003
	17	3.0969	400.35	0.0014
	18	3.1705	391.06	0.0563
	19	3.2054	386.8	0.0159
	20	3.2395	382.73	0.2929
	21	3.376	367.25	0.1361
	22	3.3922	365.5	0.0197
	23	3.5151	352.72	0.0009
	24	3.579	346.42	0.3801
	25	3.6121	343.25	0.0950

Table S13 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-BC_2O4-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-BC_2O4-e	1	2.6124	474.61	0.2841
	2	2.7428	452.03	0.1446
	3	2.8912	428.83	0.0000
	4	3.1498	393.63	0.0001
	5	3.2375	382.96	0.0025
	6	3.2954	376.24	1.1203
	7	3.4821	356.06	0.1958
	8	3.5467	349.58	0.2510
	9	3.6718	337.67	0.0032
	10	3.682	336.73	0.0072
	11	3.8434	322.59	0.0447
	12	3.8851	319.13	0.0548
	13	3.9956	310.3	0.0001
	14	3.9977	310.14	0.0003
	15	4.0089	309.27	0.0442
	16	4.0457	306.46	0.0011
	17	4.1189	301.01	0.0037
	18	4.1338	299.93	0.0022
	19	4.1414	299.38	0.0002
	20	4.1432	299.24	0.0000
	21	4.1736	297.07	0.0173
	22	4.1903	295.88	0.0001
	23	4.2287	293.2	0.0000
	24	4.2531	291.52	0.0000
	25	4.2804	289.66	0.0000

Table S14 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-$BCO_2$2-s.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-$BCO_2$2-s	1	0.1097	11301.25	0.0030
	2	1.2484	993.11	0.0105
	3	1.3576	913.25	0.0306
	4	1.4466	857.08	0.0195
	5	1.8716	662.44	0.0447
	6	2.0395	607.92	0.0026
	7	2.1135	586.63	0.0300
	8	2.4067	515.17	0.0897
	9	2.4702	501.92	0.0984
	10	2.5745	481.58	0.1352
	11	2.8622	433.19	0.0047
	12	3.2176	385.33	0.0008
	13	3.2669	379.51	0.0008
	14	3.2694	379.22	0.0092
	15	3.3493	370.18	0.2411
	16	3.3706	367.84	0.0005
	17	3.4044	364.19	0.0051
	18	3.4515	359.22	0.0079
	19	3.5148	352.75	0.0036
	20	3.5315	351.08	0.0009
	21	3.6587	338.87	0.0528
	22	3.6895	336.05	0.6066
	23	3.7806	327.94	0.4922
	24	3.7998	326.30	0.3627
	25	3.9113	316.99	0.1122

Table S15 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-$BCO_2$2-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-$BCO_2$2-e	1	2.8568	434	0.004
	2	2.9847	415.4	0.0065
	3	3.2925	376.56	0.027
	4	3.3057	375.06	0.1016
	5	3.3653	368.42	1.0086
	6	3.3728	367.6	0.9677
	7	3.528	351.43	0.002
	8	3.5575	348.52	0.0002
	9	3.8251	324.14	0.0001
	10	3.8319	323.56	0.01
	11	3.8525	321.82	0.0012
	12	4.0598	305.39	0.001
	13	4.0873	303.34	0.0017
	14	4.167	297.54	0.0004
	15	4.1816	296.5	0.0015
	16	4.2527	291.55	0.0002
	17	4.3074	287.84	0.0255
	18	4.3413	285.59	0.0062
	19	4.3686	283.81	0.0046
	20	4.3772	283.25	0.0000
	21	4.4399	279.25	0.0044
	22	4.4524	278.47	0.0007
	23	4.4742	277.11	0.0047
	24	4.4868	276.33	0.0002
	25	4.4956	275.79	0.0014

Table S16 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-B2-$BCO_2$2-s.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-B2-$BCO_2$2-s	1	1.8453	671.88	0.0233
	2	1.9663	630.53	0.0784
	3	2.0972	591.18	0.0927
	4	2.1251	583.44	0.1018
	5	2.4478	506.5	0.0080
	6	2.47	501.96	0.0085
	7	2.6059	475.78	0.0037
	8	2.7111	457.33	0.0764
	9	2.7306	454.06	0.2256
	10	2.9384	421.95	0.0260
	11	3.0185	410.74	0.2546
	12	3.1087	398.83	0.0254
	13	3.2633	379.94	0.1456
	14	3.3514	369.95	0.0219
	15	3.4368	360.75	0.0169
	16	3.446	359.79	0.0892
	17	3.4646	357.86	0.0011
	18	3.5713	347.16	0.0171
	19	3.6142	343.05	0.0020
	20	3.6854	336.42	0.1522
	21	3.6948	335.57	0.3763
	22	3.7721	328.69	0.1713
	23	3.7906	327.08	0.0923
	24	3.8038	325.95	0.0230
	25	3.8441	322.53	0.0986

Table S17 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-B2-$BCO_2$2-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-B2-$BCO_2$2-e	1	0.0992	12502.41	0.0011
	2	0.7572	1637.35	0.0068
	3	0.9571	1295.39	0.0647
	4	1.1275	1099.67	0.2235
	5	1.8358	675.35	0.0159
	6	1.9385	639.59	0.0305
	7	2.0876	593.9	0.1660
	8	2.1768	569.58	0.0249
	9	2.1878	566.72	0.0000
	10	2.3797	521.00	0.0000
	11	2.7418	452.2	0.3893
	12	2.7603	449.17	0.0002
	13	2.8942	428.39	0.0497
	14	2.9086	426.26	0.0026
	15	3.0798	402.57	0.0265
	16	3.1408	394.75	0.084
	17	3.1476	393.91	0.001
	18	3.2909	376.75	0.0786
	19	3.3887	365.88	0.1529
	20	3.4416	360.25	0.0328
	21	3.4746	356.83	0.0028
	22	3.5224	351.99	0.3613
	23	3.5614	348.13	0.0895
	24	3.6063	343.8	0.0004
	25	3.6985	335.23	0.0989

Table S18 Absorption energy, wavelengths, and oscillator strengths for the first 25 singlet states of GQD-$BCO_2$4-e.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator Strengths (f)
GQD-$BCO_2$4-e	1	2.8148	440.47	0.0175
	2	2.9392	421.83	0.0231
	3	3.2536	381.07	0
	4	3.3082	374.78	1.185
	5	3.31	374.58	0
	6	3.3275	372.6	0.9669
	7	3.5071	353.52	0
	8	3.5365	350.59	0
	9	3.7554	330.15	0.0316
	10	3.8047	325.87	0.0076
	11	3.8322	323.54	0.0001
	12	4.0259	307.96	0.0054
	13	4.0605	305.34	0.0068
	14	4.0626	305.19	0
	15	4.1677	297.49	0.0033
	16	4.2107	294.45	0
	17	4.2396	292.44	0
	18	4.2456	292.03	0.0023
	19	4.2502	291.71	0.0759
	20	4.2883	289.12	0
	21	4.3025	288.17	0
	22	4.3374	285.85	0.0278
	23	4.3804	283.05	0
	24	4.4411	279.17	0.0004
	25	4.4523	278.47	0