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

Electronic Supporting Information

Theoretical Study on Optical and Electronic Properties of Graphene Quantum Dots Doped with Heteroatoms

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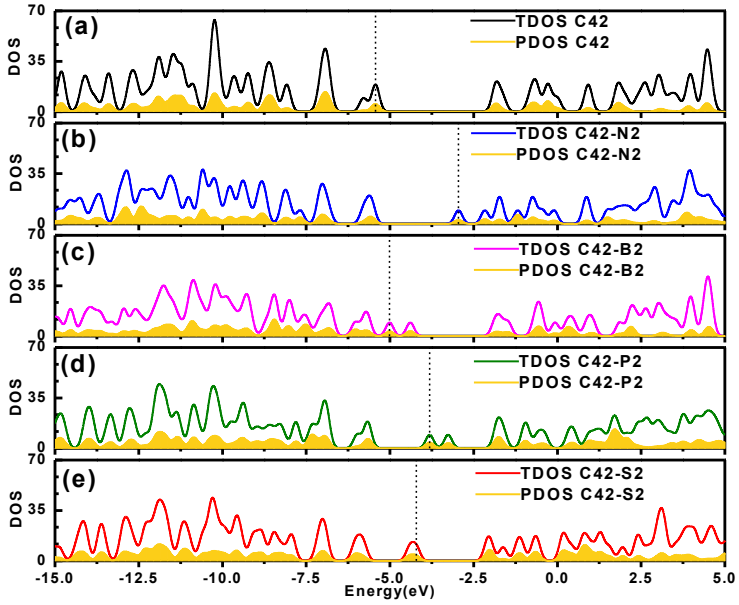

Fig. S1 Density of state of pristine GODs and doped GQDs. (a) pristine GQD, (b) C42-N2, (c) C42-B2, (d) C42-P2, and (e) C42-S2, respectively. The solid lines represent total DOS (TDOS). The yellow-filled regions represent partial DOS (PDOS) of two benzene rings in pristine GQDs for (a), and two five-member rings containing heteroatoms in doped GQDs for (b)-(e), respectively. (The vertical dashed line indicates the position of the HOMO level. The DOS is plotted with a Gaussian width of 0.01a.u.)

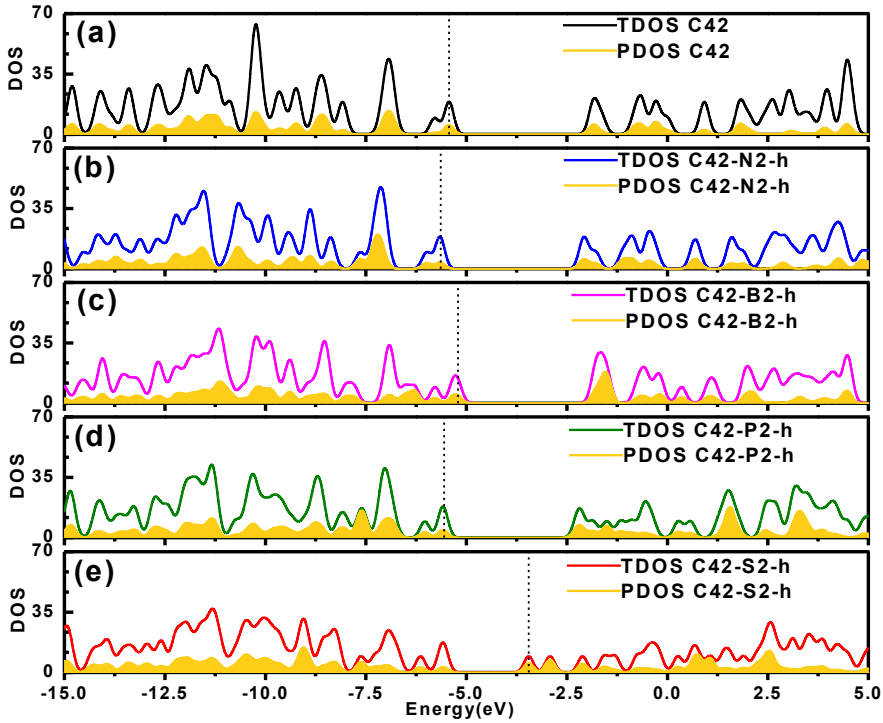

Fig. S2 Density of state of pristine GODs and doped GQDs. (a) pristine GQD, (b) C42-N2-*h*, (c) C42-B2-*h*, (d) C42-P2-*h*, and (e) C42-S2-*h*, respectively.

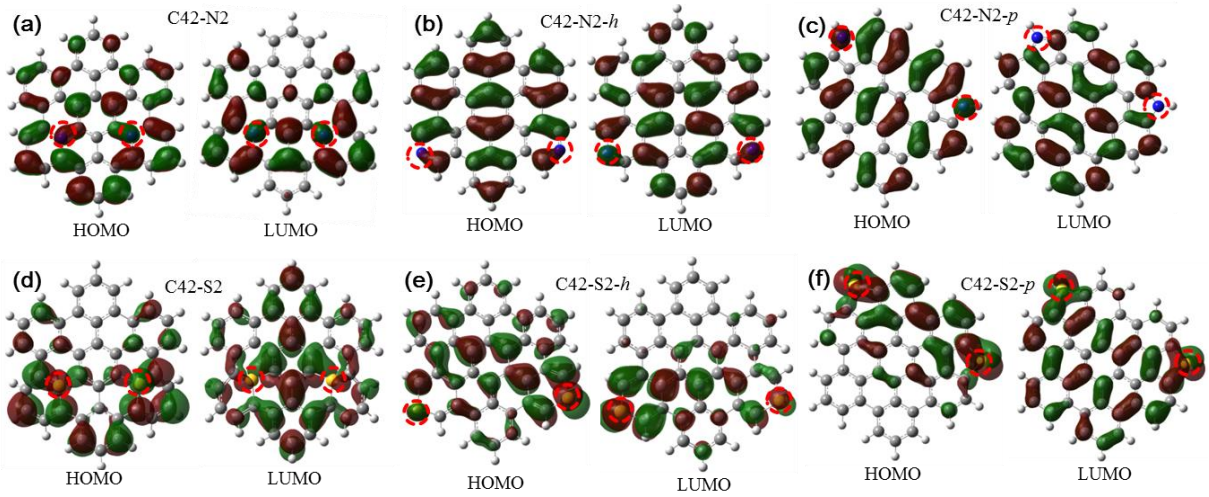

Fig. S3 Isosurfaces of HOMO and LUMO in N- and S-doped GQDs with different patterns in ground state. The positive and negative orbital lobes are displayed in red and green colors, respectively.

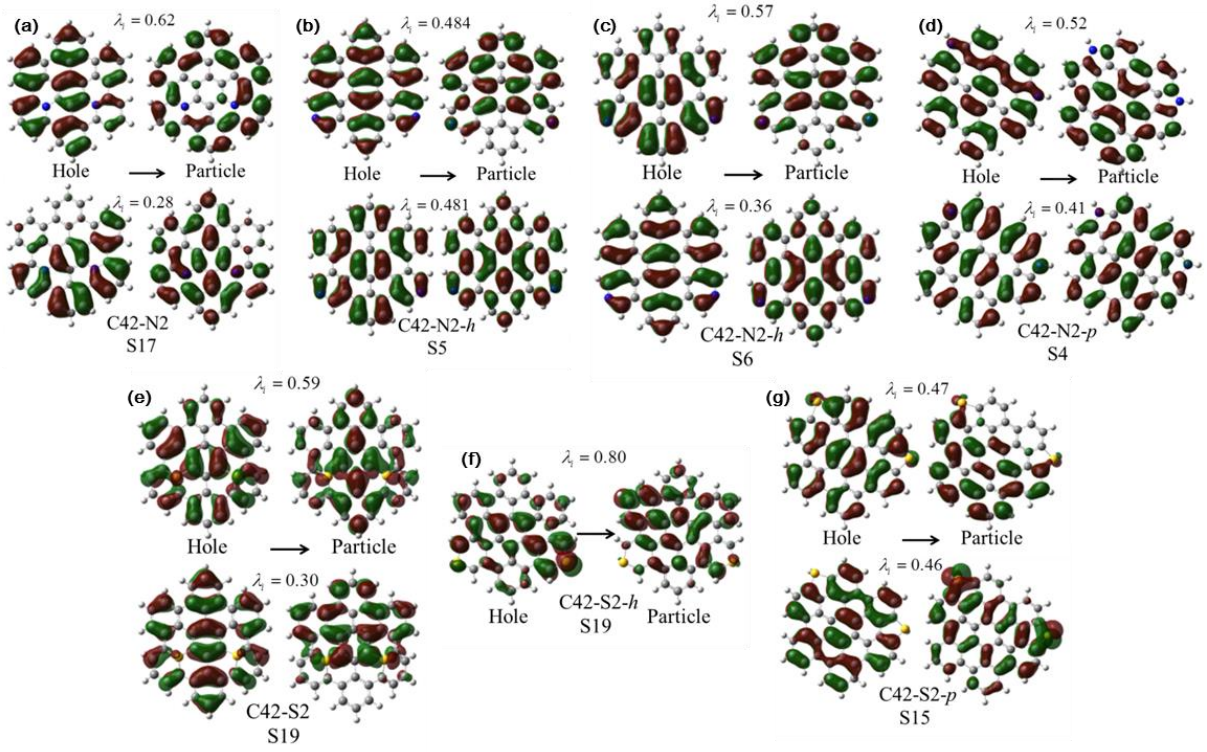

Fig. S4 The NTO pairs for the prominent excited state of N- and S-doped GQDs. For this state the "hole" is on the left, and the "particle" is on the right; the values represent the associated eigenvalue (λ_i).

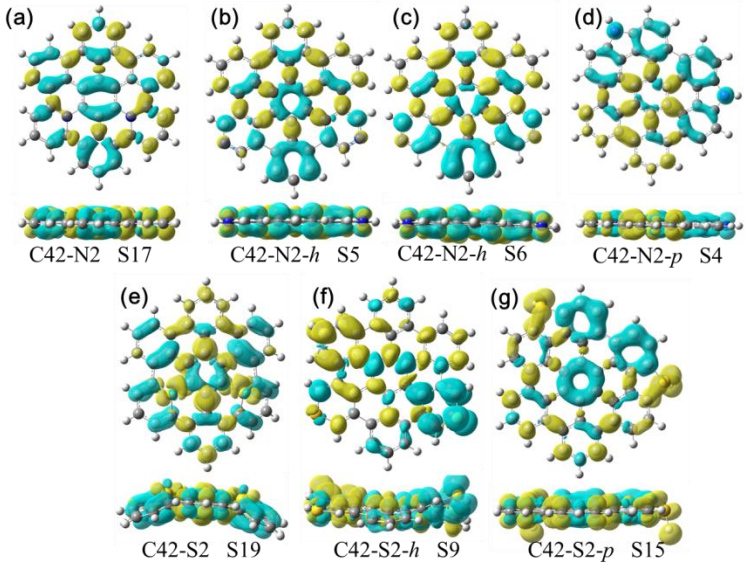

Fig. S5 Representation of the charge difference density between the prominent excited state minus ground state for N- and S-doped GQDs. Lateral views are displayed at the bottom. (The blue and yellow colors represent hole and electron, respectively. The isovalue is $4*10^{-4}$).

Table S1 The Cartesian Coordinates of stationary points for the optimized ground state geometry of C42

C42			
	X	Y	Z
C	-2.842755	4.928235	-0.00001
C	-2.860333	2.497661	-0.000002
C	-3.537311	3.726867	-0.000006
C	-4.995144	1.20438	0.000006
C	-2.87248	0.001412	0.000002
C	-3.591933	1.231772	0.000002
C	-4.996326	-1.19947	0.000008
C	-2.862787	-2.494848	0.000003
C	-3.593142	-1.228241	0.000005
C	-2.847598	-4.925439	0.000004
C	-3.540973	-3.723388	0.000005
C	1.459587	4.926826	-0.000005
C	-1.455133	4.928031	-0.000009
C	-0.728918	3.726704	-0.000006
C	1.43755	2.486983	0
C	0.732694	3.726147	-0.000004
C	-1.434999	2.488437	-0.000003
C	-0.711403	1.233826	-0.000001
C	1.424431	-0.0007	0.000001
C	0.71288	1.233274	0
C	-1.423917	0.0007	0
C	-0.712615	-1.233127	0
C	1.435104	-2.488395	-0.000002
C	0.711667	-1.233974	0
C	-1.437444	-2.487025	0
C	-0.732581	-3.725986	-0.000002
C	1.454743	-4.928258	-0.000014
C	0.729031	-3.726865	-0.000006
C	-1.459977	-4.926599	0.000001
C	3.54058	3.723962	0.000004
C	2.863012	2.494718	0.000004
C	3.59332	1.228491	0.000006
C	5.689564	-0.002796	0.000012
C	4.996596	1.199305	0.000011
C	2.872524	-0.001412	0.000003
C	3.59211	-1.232022	0.000003
C	4.995415	-1.204215	0.000008
C	2.860559	-2.49753	-0.000002
C	3.536917	-3.727441	-0.000007
H	-4.619123	3.760836	-0.000006
H	-5.564785	2.124754	0.000006
H	-5.56687	-2.119283	0.000011
H	-4.622818	-3.756294	0.000007
C	-5.689425	0.002796	0.000009
H	-6.775459	0.00333	0.000012
C	2.842247	-4.92863	-0.000014
C	2.847091	4.925834	-0.000001
H	-3.38568	5.868839	-0.000013
H	-0.943163	5.881537	-0.000012
H	0.948606	5.880843	-0.000009
H	3.390482	5.866183	-0.000001
H	4.622261	3.757177	0.000007
H	5.567361	2.118782	0.000013
H	6.775623	-0.00333	0.000015
H	5.565276	-2.124252	0.000008
H	4.618565	-3.761719	-0.000007
H	3.384714	-5.869513	-0.00002
H	0.942825	-5.881773	-0.00002
H	-0.948944	-5.880607	0.000001
H	-3.391448	-5.865508	0.000006

Table S2 The Cartesian Coordinates of stationary points for the optimized ground state geometry of N-GQDs

C42-N2				C42-N2-*h*				C42-N2-*p*			
	X	Y	Z		X	Y	Z		X	Y	Z
C	5.700788	-0.011712	0.000017	**C**	2.856921	-2.480537	-0.000025	**C**	-2.87629	5.046505	0.000008
C	3.600239	-1.238223	0.000004	**C**	3.494358	-3.729741	-0.000052	**C**	-0.742873	3.865281	0.000003
C	5.006898	-1.213053	0.000011	**C**	4.999683	-1.192608	-0.000015	**C**	-1.482832	5.059276	0.000007
C	3.538122	-3.740288	-0.000006	**C**	2.875214	0.007006	-0.000003	**C**	1.480571	5.059946	-0.00001
C	1.448649	-2.475257	-0.000004	**C**	3.597068	-1.221873	-0.000015	**C**	1.466746	2.632755	0.000002
C	2.869755	-2.496477	-0.000002	**C**	4.99408	1.216353	0.000005	**C**	0.741192	3.865628	-0.000002
C	1.436539	-4.907786	-0.000013	**C**	2.844991	2.494501	0.000015	**C**	3.582752	3.849305	-0.000007
C	-0.735551	-3.684012	-0.00001	**C**	3.591253	1.23921	0.000006	**C**	3.63012	1.331115	0.000001
C	0.733826	-3.701392	-0.000009	**C**	3.476222	3.746918	0.000027	**C**	2.91394	2.617211	-0.000001
C	-2.858583	-4.889374	-0.000019	**C**	-1.424904	-4.934127	0.000066	**C**	5.634796	-0.191462	-0.000006
C	-1.452478	-4.857126	-0.000017	**C**	1.520841	-4.878848	-0.000037	**C**	5.038508	1.089325	-0.000004
C	3.553592	3.725767	0.000012	**C**	0.749014	-3.707492	-0.000005	**C**	-2.914965	2.616067	0.000002
C	5.011899	1.192464	0.000015	**C**	-1.424811	-2.492387	0.000016	**C**	-2.825031	0.179164	0.000004
C	3.605314	1.223438	0.000009	**C**	-0.710642	-3.727415	0.000025	**C**	-3.630511	1.32962	-0.000001
C	1.458896	2.469331	0	**C**	1.43807	-2.468253	-0.000008	**C**	-1.467802	2.632098	0.000003
C	2.880053	2.484687	0.000007	**C**	0.711723	-1.223401	0	**C**	-0.711028	1.406258	0.000005
C	1.425346	-0.002889	0	**C**	-1.427114	-0.003455	0	**C**	-0.695368	-1.064919	0.000009
C	-0.705218	1.235308	-0.000003	**C**	-0.710284	-1.233024	0.000003	**C**	-1.398048	0.173903	0.000007
C	0.729674	1.233431	-0.000002	**C**	1.426217	0.00349	0	**C**	0.710457	1.40657	0.000006
C	0.724542	-1.236411	-0.000002	**C**	0.70582	1.226927	0.000003	**C**	1.398086	0.174426	0.000008
C	-0.710285	-1.232362	-0.000002	**C**	-1.436888	2.485466	-0.000003	**C**	1.353187	-2.34199	0.000007
C	-2.864359	0.005868	0.000009	**C**	-0.716254	1.229604	0	**C**	0.695844	-1.064722	0.00001
C	-1.427852	0.002929	0	**C**	1.426126	2.475211	0.00001	**C**	2.824977	0.180132	0.000006
C	-2.840896	-2.453032	0.000002	**C**	0.731051	3.711165	0.000015	**C**	3.433648	-1.065317	0.000005
C	-4.997816	-1.201139	0.000036	**C**	-1.449073	4.927125	0.000004	**C**	3.640373	-3.327941	0
C	-3.57428	-1.227914	0.000016	**C**	-0.728816	3.723935	0.000006	**C**	2.734815	-2.269481	0.000007
C	-3.515305	-3.690535	-0.000009	**C**	1.497137	4.886296	0.000029	**C**	4.800685	-1.331681	-0.000002
C	1.456794	4.901865	0.000003	**C**	-3.516298	-3.741178	0.000064	**C**	-4.800129	-1.333417	-0.000006
C	0.749101	3.698404	-0.000003	**C**	-2.849359	-2.505727	0.000026	**C**	-3.433164	-1.066566	0.000002
C	-0.720324	3.687008	-0.000015	**C**	-3.586687	-1.241047	-0.000004	**C**	-2.733862	-2.270418	0.000004
C	-2.838362	4.901142	-0.000041	**C**	-4.989724	-1.215532	-0.00003	**C**	-3.055739	-4.615139	-0.000007
C	-1.432433	4.863049	-0.000033	**C**	-2.873191	-0.006997	-0.000008	**C**	-3.638993	-3.329254	-0.000004
C	-2.830776	2.464713	-0.000006	**C**	-3.59264	1.223592	-0.000026	**C**	-1.35215	-2.342436	0.000007
C	-3.499987	3.704932	-0.000026	**C**	-4.995515	1.191375	-0.000053	**C**	-0.737254	-3.624637	0.000004
C	-3.569254	1.242556	0.000012	**C**	-2.861504	2.491829	-0.000015	**C**	-1.645285	-4.725915	-0.000001
C	-4.992792	1.221526	0.000031	**C**	-3.534555	3.723944	-0.000014	**C**	0.738632	-3.624409	0.000004
H	5.573572	-2.135262	0.000012	**H**	4.577402	-3.798722	-0.000072	**C**	1.647153	-4.725379	-0.000001
H	4.61998	-3.780488	-0.000005	**H**	5.569629	-2.113436	-0.00002	**H**	-0.980609	6.019552	0.000012
H	0.920662	-5.858479	-0.000016	**H**	5.559876	2.139712	0.000012	**H**	0.977943	6.019999	-0.000018
H	-0.916015	-5.793605	-0.000024	**H**	4.558859	3.821542	0.000032	**H**	4.668116	3.874637	-0.000009
C	2.834205	-4.927212	-0.000011	**H**	1.046478	-5.854931	-0.000049	**H**	5.719302	1.935732	-0.000008
H	3.359478	-5.877414	-0.000014	**H**	-0.903879	-5.883396	0.000087	**C**	2.874106	5.047739	-0.000013
C	-5.667766	0.011534	0.000043	**H**	-4.597872	-3.782893	0.000082	**H**	3.414394	5.990277	-0.000019
C	2.854559	4.91553	0.000011	**H**	-5.558461	-2.136523	-0.000036	**C**	3.057557	-4.61407	-0.000004
H	6.787347	-0.013987	0.000022	**H**	-5.568594	2.109663	-0.000075	**C**	-5.634663	-0.193497	-0.000011
H	5.582333	2.112339	0.00002	**H**	-4.616324	3.76026	-0.000019	**H**	-3.416896	5.98886	0.000011
H	4.6356	3.761467	0.000017	**H**	-0.932742	5.878923	0.000009	**H**	-6.717884	-0.267936	-0.000018
H	3.383711	5.863579	0.000016	**H**	1.018099	5.860069	0.000037	**H**	-3.652335	-5.522374	-0.000012
H	0.944873	5.854691	0.000004	**N**	2.831995	4.91659	0.000036	**H**	-1.238161	-5.733799	0
H	-0.89207	5.797293	-0.000042	**C**	-2.837789	4.924995	-0.000006	**H**	1.240361	-5.733415	-0.000004
H	-3.369729	5.845821	-0.000057	**H**	-3.3809	5.865338	-0.000006	**H**	3.65436	-5.521205	-0.000009
H	-4.579447	3.698021	-0.000031	**C**	-2.813605	-4.938784	0.000087	**H**	6.718043	-0.265308	-0.000011
H	-5.569104	2.135446	0.00004	**H**	-3.352041	-5.881808	0.000123	**H**	5.798499	-3.244727	-0.000005
H	-6.755373	0.013803	0.00006	**C**	-5.68484	-0.013743	-0.000057	**N**	4.924963	-2.738304	-0.000005
H	-5.577766	-2.112746	0.000049	**H**	-6.770798	-0.016343	-0.000082	**H**	-5.797214	-3.246773	-0.000017
H	-4.59472	-3.679124	-0.000011	**N**	2.855794	-4.902433	-0.000062	**N**	-4.923854	-2.740046	-0.000009
H	-3.393828	-5.831867	-0.000028	**C**	5.689024	0.013475	-0.000005	**C**	-5.038791	1.087496	-0.000008
N	-1.404921	2.440539	-0.000008	**H**	6.774835	0.015949	-0.000004	**C**	-3.5844	3.847621	0.000004
N	-1.415014	-2.434807	-0.000003					**H**	-4.669732	3.872458	0.000004
C	2.878863	-0.005889	0.000004					**H**	-5.719753	1.933717	-0.000013

Table S3 The Cartesian Coordinates of stationary points for the optimized ground state geometry of B-GQDs

C42-B2				C42-B2-*h*				C42-B2-*p*			
	X	Y	Z		X	Y	Z		X	Y	Z
C	5.689167	0.152664	-0.003542	**C**	2.944035	-2.506833	-0.000135	**C**	-2.865474	5.014704	0.000034
C	3.565562	1.332765	-0.001306	**C**	3.719507	-3.700545	-0.000274	**C**	-0.738109	3.824248	0.000007
C	4.967786	1.339056	-0.002758	**C**	5.05921	-1.195801	-0.000038	**C**	-1.475208	5.021542	0.000026
C	3.447822	3.814059	0.000217	**C**	2.928772	0.000131	-0.000004	**C**	1.474162	5.021806	-0.000024
C	1.361993	2.535466	0.000106	**C**	3.656064	-1.225516	-0.000061	**C**	1.455339	2.591832	-0.000004
C	2.789977	2.576276	-0.000367	**C**	5.059188	1.196096	0.000057	**C**	0.737271	3.824401	-0.000006
C	1.37724	5.01743	0.001462	**C**	2.943886	2.507112	0.000098	**C**	3.567779	3.81398	-0.000022
C	-0.787652	3.827372	0.001347	**C**	3.656019	1.225817	0.000051	**C**	3.618933	1.307841	-0.000003
C	0.638986	3.801724	0.000992	**C**	3.719292	3.700968	0.000182	**C**	2.893642	2.586297	-0.000009
C	-2.964871	4.904226	0.00269	**C**	-1.441294	-4.924098	0.000243	**C**	5.647495	-0.113579	-0.000001
C	-1.587807	5.004302	0.002561	**C**	1.403592	-5.02915	-0.000204	**C**	5.02218	1.150375	-0.000004
C	3.647344	-3.623662	0.001684	**C**	0.764482	-3.7577	-0.000061	**C**	-2.894192	2.585824	0.000008
C	5.032443	-1.070722	-0.002642	**C**	-1.389325	-2.484835	0.000058	**C**	-2.839837	0.120209	0
C	3.631903	-1.139612	-0.001035	**C**	-0.701465	-3.730166	0.000082	**C**	-3.619242	1.30709	0
C	1.496015	-2.458684	0.000419	**C**	1.501431	-2.514731	-0.00006	**C**	-1.455908	2.591529	0.000004
C	2.924114	-2.422939	0.000323	**C**	0.777257	-1.247621	-0.000011	**C**	-0.709375	1.354656	0.000002
C	1.448527	0.038899	-0.000195	**C**	-1.361104	-0.000053	-0.000004	**C**	-0.699809	-1.109794	0.000004
C	-0.671897	-1.242332	-0.000226	**C**	-0.651871	-1.237339	0.000005	**C**	-1.405075	0.121642	0.000003
C	0.752157	-1.215166	-0.000069	**C**	1.481571	0.000085	-0.000003	**C**	0.709023	1.354793	0.000002
C	0.685922	1.253774	-0.000066	**C**	0.777165	1.247733	0.000012	**C**	1.40514	0.121885	0.000004
C	-0.737495	1.204516	-0.000112	**C**	-1.38955	2.484719	-0.000031	**C**	1.385947	-2.378502	0.000006
C	-2.938196	-0.078847	-0.000807	**C**	-0.651973	1.237303	-0.000007	**C**	0.700017	-1.109766	0.000005
C	-1.434374	-0.038519	-0.000322	**C**	1.501254	2.514922	0.000053	**C**	2.839734	0.120724	0.000003
C	-3.042013	2.442964	0.000159	**C**	0.764122	3.75781	0.000065	**C**	3.494254	-1.106053	0.000006
C	-5.114596	1.061247	-0.002462	**C**	-1.441736	4.923994	-0.000063	**C**	3.623254	-3.469778	0.000011
C	-3.711979	1.130739	-0.000949	**C**	-0.701805	3.730123	-0.00001	**C**	2.771659	-2.348151	0.000009
C	-3.68772	3.661193	0.001529	**C**	1.403073	5.029413	0.000149	**C**	4.88838	-1.293064	0.000005
C	1.644182	-4.936279	0.002326	**C**	-3.506592	-3.710744	0.000257	**C**	-4.888111	-1.293996	-0.000011
C	0.841919	-3.761876	0.001227	**C**	-2.81543	-2.490171	0.000111	**C**	-3.494013	-1.106634	-0.000004
C	-0.581173	-3.864054	0.000951	**C**	-3.540694	-1.225077	0.000014	**C**	-2.771335	-2.348662	-0.000003
C	-2.697216	-5.056355	0.00127	**C**	-4.944287	-1.19905	-0.000051	**C**	-2.975251	-4.712065	-0.000011
C	-1.31677	-5.082287	0.00155	**C**	-2.814242	-0.00013	-0.000023	**C**	-3.622355	-3.470229	-0.00001
C	-2.906771	-2.602722	-0.000465	**C**	-3.540823	1.224745	-0.000087	**C**	-1.385393	-2.378789	0.000002
C	-3.48596	-3.854076	0.000344	**C**	-4.94442	1.198539	-0.000146	**C**	-0.735617	-3.654392	0.000001
C	-3.646122	-1.328199	-0.00138	**C**	-2.815659	2.489924	-0.000085	**C**	-1.563908	-4.792965	-0.000006
C	-5.050482	-1.333708	-0.002781	**C**	-3.506911	3.710453	-0.000125	**C**	0.736111	-3.654469	0.000005
H	5.520615	2.269293	-0.0035	**H**	4.795559	-3.692026	-0.000356	**C**	1.564862	-4.79287	0.000007
H	4.5291	3.856966	0.000061	**H**	5.635809	-2.109723	-0.000057	**H**	-0.969203	5.979272	0.000038
H	0.84289	5.959781	0.002089	**H**	5.635795	2.110002	0.000092	**H**	0.968023	5.979453	-0.000036
H	-1.15519	6.001584	0.003524	**H**	4.795324	3.692431	0.000229	**H**	4.651892	3.839469	-0.000027
C	2.752925	5.027168	0.001105	**H**	0.851237	-5.952823	-0.000251	**H**	5.661164	2.027277	-0.000008
H	3.301495	5.963904	0.001515	**H**	-0.946838	-5.885273	0.00032	**C**	2.864471	5.015195	-0.000031
C	-5.783091	-0.154994	-0.00345	**H**	-4.588106	-3.732814	0.000329	**H**	3.405366	5.956826	-0.000045
C	3.018415	-4.872282	0.002681	**H**	-5.51351	-2.118966	-0.00005	**C**	2.976369	-4.711535	0.00001
H	6.774712	0.181713	-0.004876	**H**	-5.513761	2.118376	-0.000207	**C**	-5.647522	-0.114794	-0.000014
H	5.634448	-1.969941	-0.003427	**H**	-4.588423	3.732449	-0.000162	**H**	-3.406507	5.956267	0.000049
H	4.729338	-3.608605	0.002154	**H**	-0.947355	5.885206	-0.000066	**H**	-6.734579	-0.148506	-0.000021
H	3.61632	-5.778339	0.003715	**H**	0.85046	5.95292	0.000176	**H**	-3.541926	-5.640212	-0.000017
H	1.161024	-5.905942	0.00301	**C**	-2.827194	4.91779	-0.00012	**H**	-1.109948	-5.779316	-0.000008
H	-0.830979	-6.054768	0.002248	**H**	-3.376095	5.854826	-0.000158	**H**	1.111472	-5.779495	0.000007
H	-3.233972	-6.002173	0.001801	**C**	-2.82676	-4.918019	0.000338	**H**	3.542953	-5.63977	0.000011
H	-4.564896	-3.999696	0.000441	**H**	-3.375568	-5.85511	0.000472	**H**	6.734552	-0.14691	-0.000002
H	-5.581094	-2.279216	-0.003525	**C**	-5.640357	-0.000296	-0.000134	**H**	6.12544	-3.465523	0.000013
H	-6.869522	-0.18404	-0.004684	**H**	-6.726446	-0.00036	-0.000189	**B**	5.093108	-2.864865	0.000009
H	-5.694953	1.977145	-0.003002	**C**	5.756244	0.000154	0.000018	**H**	-6.124527	-3.467033	-0.000028
H	-4.772991	3.748173	0.002	**H**	6.842095	0.00015	0.000032	**B**	-5.092349	-2.866121	-0.000017
H	-3.551677	5.819851	0.003724	**B**	2.799123	4.779844	0.000191	**C**	-5.022383	1.149358	-0.000008
B	-1.38949	-2.562328	-0.000032	**B**	2.799636	-4.779644	-0.000289	**C**	-3.568533	3.813236	0.000023
B	-1.524811	2.484093	0.000289					**H**	-4.6526	3.838624	0.00003
C	2.884589	0.077391	-0.000767					**H**	-5.661603	2.02603	-0.000012

Table S4 The Cartesian Coordinates of stationary points for the optimized ground state geometry of P-GQDs

C42-P2				C42-P2-*h*				C42-P2-*p*			
	X	Y	Z		X	Y	Z		X	Y	Z
C	-0.341592	5.771513	-0.238867	**C**	-2.437685	-2.73058	-0.206753	**C**	-2.860973	5.215658	-0.000007
C	1.014079	3.754963	-0.214834	**C**	-3.553533	-3.488102	-0.583647	**C**	-0.735765	4.02699	-0.000004
C	0.894144	5.147479	-0.338619	**C**	-1.167361	-4.793413	0.392262	**C**	-1.469007	5.223131	-0.000003
C	3.497578	3.886592	-0.208694	**C**	0.037711	-2.691144	0.136392	**C**	1.470562	5.222611	0.000011
C	2.423938	1.681903	-0.204615	**C**	-1.181842	-3.421547	0.104598	**C**	1.449855	2.789264	0.000001
C	2.326743	3.101756	-0.229573	**C**	1.2263	-4.756644	0.616583	**C**	0.736824	4.026791	0.000002
C	4.875976	1.929549	-0.101	**C**	2.538759	-2.654905	0.215875	**C**	3.562004	4.015067	0.000023
C	3.939958	-0.338849	-0.023168	**C**	1.265485	-3.382366	0.328221	**C**	3.605119	1.513222	0.000012
C	3.745886	1.097453	-0.116711	**C**	3.734175	-3.38531	0.253098	**C**	2.885414	2.784494	0.000013
C	4.999088	-2.394391	0.845433	**C**	-4.931924	1.516759	0.343054	**C**	5.68037	0.169441	0.000042
C	4.993849	-1.003738	0.580032	**C**	-4.906928	-1.224196	-0.58013	**C**	5.020892	1.393677	0.000044
C	-3.896743	3.469757	0.393118	**C**	-3.712032	-0.596216	-0.206166	**C**	-2.884819	2.78528	-0.00001
C	-1.486633	5.021184	-0.010996	**C**	-2.504338	1.561059	0.154145	**C**	-2.850336	0.320294	-0.000006
C	-1.429907	3.622301	0.094284	**C**	-3.727896	0.840234	0.09697	**C**	-3.604963	1.514108	-0.000009
C	-2.58511	1.402509	0.258706	**C**	-2.472693	-1.304896	-0.120063	**C**	-1.449161	2.789753	-0.000008
C	-2.648585	2.82488	0.267366	**C**	-1.22899	-0.565776	0.005329	**C**	-0.712344	1.549661	-0.00001
C	-0.081827	1.53573	0.004022	**C**	-0.027349	1.586116	0.035628	**C**	-0.704739	-0.919576	-0.00001
C	-1.122846	-0.654541	0.263075	**C**	-1.246737	0.856805	0.052243	**C**	-1.412731	0.317343	-0.000009
C	-1.264813	0.749626	0.169341	**C**	0.020816	-1.251947	0.031197	**C**	0.712625	1.549415	-0.000009
C	1.182536	0.886741	-0.156579	**C**	1.247982	-0.528518	0.011473	**C**	1.412612	0.316984	-0.000018
C	1.200019	-0.522816	-0.268411	**C**	2.439576	1.644936	-0.187438	**C**	1.396174	-2.182439	-0.000017
C	0.158115	-2.843734	-0.033066	**C**	1.214999	0.895616	-0.03146	**C**	0.70441	-0.919788	-0.000018
C	0.079163	-1.342111	-0.01292	**C**	2.520162	-1.232111	0.043344	**C**	2.850316	0.319784	-0.000014
C	2.68102	-2.83532	0.132843	**C**	3.739198	-0.488069	-0.080953	**C**	3.516317	-0.922419	-0.000031
C	1.454583	-4.944958	0.107928	**C**	4.822971	1.694532	-0.670286	**C**	3.58712	-3.331564	-0.000009
C	1.41456	-3.536293	0.105902	**C**	3.678198	0.961188	-0.319081	**C**	2.803706	-2.151889	-0.00003
C	3.875808	-3.235727	0.715423	**C**	4.998642	-1.08786	0.044794	**C**	4.929227	-1.02034	-0.000007
C	-5.051165	1.371596	0.340402	**C**	-3.761223	3.606945	0.568688	**C**	-4.929496	-1.019223	0.000003
C	-3.837109	0.675537	0.246927	**C**	-2.529425	2.972222	0.347092	**C**	-3.516637	-0.921744	0.000002
C	-3.876736	-0.771377	0.112207	**C**	-1.279291	3.726737	0.290949	**C**	-2.804201	-2.15178	0.000005
C	-4.729227	-2.900986	-0.801622	**C**	-1.263468	5.125858	0.401799	**C**	-2.924783	-4.57301	0.000015
C	-4.87211	-1.528479	-0.480069	**C**	-0.051103	3.032725	0.094364	**C**	-3.587866	-3.331094	0.000011
C	-2.352891	-3.104054	-0.177346	**C**	1.157665	3.774337	-0.025356	**C**	-1.396719	-2.182097	0
C	-3.516499	-3.614935	-0.73852	**C**	1.123973	5.170689	0.106494	**C**	-0.728507	-3.435804	0.000007
C	-1.017708	-3.662883	-0.196378	**C**	2.409682	3.066257	-0.2748	**C**	-1.534518	-4.606123	0.000014
C	-0.904258	-5.066218	-0.258789	**C**	3.585221	3.756518	-0.603793	**C**	0.727864	-3.436059	0.000005
H	1.763871	5.763771	-0.524797	**H**	-3.416912	-4.556113	-0.714715	**C**	1.533719	-4.606479	0.000033
H	3.430641	4.966214	-0.21069	**H**	-2.093444	-5.352202	0.448352	**H**	-0.962511	6.180387	0.000002
H	5.860936	1.475762	-0.070088	**H**	2.133324	-5.303939	0.835973	**H**	0.964426	6.180064	0.00001
H	5.824942	-0.427248	0.982935	**H**	3.670626	-4.46426	0.321508	**H**	4.645692	4.041619	0.000029
C	4.757252	3.311352	-0.153663	**H**	-5.785122	-0.601076	-0.708854	**H**	5.634785	2.287608	0.000078
H	5.643673	3.938782	-0.147233	**H**	-5.869181	0.975531	0.378904	**C**	2.862551	5.214673	0.000021
C	0.313934	-5.710652	-0.092378	**H**	-3.806246	4.674202	0.74465	**H**	3.404922	6.155871	0.000027
C	-5.083072	2.756216	0.440123	**H**	-2.183881	5.676434	0.549626	**C**	2.924028	-4.573407	0.000033
H	-0.413218	6.850372	-0.340704	**H**	2.039138	5.748081	0.060418	**C**	-5.680465	0.17059	-0.000004
H	-2.431118	5.544506	0.054905	**H**	3.573163	4.83256	-0.725246	**H**	-3.403045	6.157033	-0.000007
H	-3.949785	4.548186	0.457039	**H**	5.763502	1.193648	-0.860121	**H**	-6.765539	0.147137	-0.000005
H	-6.0297	3.277337	0.548275	**H**	5.870076	-0.444157	0.029768	**H**	-3.482603	-5.50411	0.000019
H	-5.977483	0.807446	0.370308	**P**	5.349493	-2.771292	0.22253	**H**	-1.055646	-5.579998	0.000017
H	-5.776451	-1.034861	-0.832226	**C**	4.77374	3.073896	-0.823896	**H**	1.054851	-5.580361	0.000063
H	-5.57167	-3.389433	-1.282099	**H**	5.667284	3.618055	-1.114757	**H**	3.481878	-5.504477	0.000059
H	-3.48338	-4.573295	-1.254534	**C**	-4.946159	2.884029	0.587627	**H**	6.765444	0.145801	0.000071
H	-1.806823	-5.656465	-0.376945	**H**	-5.886169	3.388396	0.79048	**H**	6.463139	-3.453178	0.000117
H	0.373278	-6.794277	-0.116144	**C**	-0.074293	5.838418	0.322013	**P**	5.258666	-2.756452	-0.000061
H	2.416154	-5.437506	0.207169	**H**	-0.082323	6.919485	0.424699	**H**	-6.464339	-3.451947	0.000006
H	3.932235	-4.209219	1.200443	**P**	-5.146018	-2.903181	-0.929451	**C**	-5.020718	1.394689	-0.000009
H	5.875662	-2.803745	1.338602	**C**	0.024868	-5.449372	0.666681	**C**	-3.560829	4.016302	-0.000011
C	-0.165634	2.976503	-0.030366	**H**	0.018928	-6.504998	0.920586	**H**	-4.644482	4.043391	-0.000013
P	-2.503267	-1.643147	0.850233					**H**	-5.634542	2.288646	-0.000013
P	2.698977	-1.331839	-0.846494					**P**	-5.259681	-2.755537	0.000013

Table S5 The Cartesian Coordinates of stationary points for the optimized ground state geometry of S-GQDs

C42-S2				C42-S2-*h*				C42-S2-*p*			
	X	Y	Z		X	Y	Z		X	Y	Z
C	-5.749605	-0.036806	0.626489	**C**	2.373581	-2.772681	0.222365	**C**	-2.867294	5.244367	-0.017064
C	-3.69005	-1.254003	0.202774	**C**	3.409296	-3.534423	0.674711	**C**	-0.73632	4.061531	-0.001673
C	-5.066442	-1.237442	0.473465	**C**	1.095588	-4.766671	-0.596328	**C**	-1.475914	5.255518	-0.01083
C	-3.680374	-3.684528	-0.299989	**C**	-0.085626	-2.671294	-0.200409	**C**	1.477786	5.255042	-0.011149
C	-1.543195	-2.517741	-0.008947	**C**	1.127275	-3.428434	-0.208225	**C**	1.45224	2.823464	0.003301
C	-2.967701	-2.506848	-0.018972	**C**	-1.306643	-4.706339	-0.783859	**C**	0.737793	4.061293	-0.001753
C	-1.627064	-4.912721	-0.54813	**C**	-2.562366	-2.595713	-0.255647	**C**	3.568296	4.040009	-0.017969
C	0.574353	-3.870226	-0.27186	**C**	-1.323075	-3.342361	-0.418526	**C**	3.612535	1.531559	-0.010737
C	-0.864651	-3.761759	-0.27278	**C**	-3.758743	-3.30071	-0.264904	**C**	2.891299	2.813419	-0.009097
C	2.796896	-4.743615	-0.948849	**C**	4.941346	1.394489	-0.525172	**C**	5.65716	0.122024	-0.051558
C	1.39639	-4.792271	-0.893356	**C**	4.833385	-1.248389	0.704269	**C**	5.0175	1.380689	-0.044817
C	-3.727266	3.637462	-0.298504	**C**	3.700325	-0.643234	0.253376	**C**	-2.89028	2.814278	-0.008853
C	-5.081813	1.172545	0.47436	**C**	2.531155	1.527143	-0.194472	**C**	-2.827834	0.353169	0.014612
C	-3.705786	1.206824	0.2035	**C**	3.742756	0.77352	-0.173928	**C**	-3.61196	1.532713	-0.010719
C	-1.575306	2.497938	-0.008424	**C**	2.413518	-1.319084	0.163059	**C**	-1.451142	2.823896	0.003322
C	-2.999553	2.468871	-0.017971	**C**	1.231421	-0.583208	0.033761	**C**	-0.70654	1.591767	0.01871
C	-1.547754	-0.009838	0.063222	**C**	0.072197	1.607713	-0.016089	**C**	-0.703117	-0.889447	0.03133
C	0.554787	1.177468	0.289079	**C**	1.262981	0.867618	-0.036164	**C**	-1.40396	0.353584	0.024956
C	-0.843195	1.23081	0.12436	**C**	-0.046861	-1.245708	-0.037432	**C**	0.707235	1.591511	0.018866
C	-0.82739	-1.241401	0.124153	**C**	-1.253961	-0.486108	-0.006347	**C**	1.404185	0.353157	0.02547
C	0.569792	-1.170246	0.289016	**C**	-2.389452	1.700536	0.227815	**C**	1.383172	-2.157857	0.02199
C	2.832656	0.018193	0.389915	**C**	-1.197657	0.946485	0.062168	**C**	0.702912	-0.8897	0.031737
C	1.343145	0.008613	0.316191	**C**	-2.521277	-1.158211	-0.047613	**C**	2.828014	0.352257	0.015325
C	2.978815	-2.501121	0.111913	**C**	-3.73241	-0.395385	0.10687	**C**	3.47186	-0.897184	0.035952
C	4.998626	-1.167312	0.374547	**C**	-4.790936	1.796199	0.693481	**C**	3.593228	-3.26929	-0.078216
C	3.590014	-1.202574	0.322556	**C**	-3.652441	1.041638	0.35151	**C**	2.771995	-2.119257	0.034406
C	3.500757	-3.59012	-0.557184	**C**	-4.995749	-0.984226	0.000561	**C**	4.863618	-1.013476	0.003609
C	-1.689862	4.891737	-0.547375	**C**	3.830751	3.523075	-0.73345	**C**	-4.863966	-1.012316	0.003467
C	-0.912805	3.750517	-0.272451	**C**	2.589619	2.933279	-0.420733	**C**	-3.472008	-0.89613	0.034852
C	0.524738	3.877192	-0.27218	**C**	1.36441	3.718494	-0.310939	**C**	-2.772674	-2.11815	0.03245
C	2.735733	4.778244	-0.950856	**C**	1.377494	5.123196	-0.403566	**C**	-2.952215	-4.540638	-0.114727
C	1.334725	4.808976	-0.894869	**C**	0.121954	3.053431	-0.085471	**C**	-3.595055	-3.267766	-0.082595
C	2.946598	2.539173	0.111796	**C**	-1.074228	3.81854	0.0552	**C**	-1.383942	-2.15743	0.021091
C	3.454381	3.634224	-0.558364	**C**	-1.007894	5.213515	-0.067226	**C**	-0.706768	-3.432836	-0.029857
C	3.574362	1.248519	0.322521	**C**	-2.343085	3.13132	0.313305	**C**	-1.574368	-4.604148	-0.096168
C	4.983332	1.2312	0.374507	**C**	-3.506658	3.830675	0.638587	**C**	0.705421	-3.433131	-0.029399
H	-5.608445	-2.166331	0.602905	**H**	3.326953	-4.610531	0.76836	**C**	1.572463	-4.604709	-0.095761
H	-4.761738	-3.668683	-0.348517	**H**	2.020454	-5.324359	-0.695191	**H**	-0.972136	6.214766	-0.013557
H	-1.11653	-5.853168	-0.725453	**H**	-2.223847	-5.228217	-1.027773	**H**	0.974316	6.21445	-0.013783
H	0.898776	-5.575344	-1.461832	**H**	-3.778769	-4.379082	-0.339065	**H**	4.652642	4.063838	-0.023474
C	-3.013238	-4.873329	-0.567287	**H**	5.769781	-0.71493	0.808228	**H**	5.656435	2.256304	-0.074337
H	-3.577248	-5.776124	-0.784108	**H**	5.854441	0.812078	-0.590988	**C**	2.869137	5.243464	-0.017722
C	5.685485	0.036378	0.419794	**H**	3.893909	4.584114	-0.944437	**H**	3.413542	6.18329	-0.023666
C	-3.07545	4.834698	-0.565906	**H**	2.309668	5.653608	-0.556251	**C**	2.950478	-4.541738	-0.113292
H	-6.80875	-0.04365	0.866297	**H**	-1.908225	5.813095	-0.002007	**C**	-5.656941	0.123613	-0.050789
H	-5.635497	2.0944	0.604501	**H**	-3.479541	4.907781	0.757334	**H**	-3.411396	6.184374	-0.022747
H	-4.808368	3.607917	-0.346635	**H**	-5.742733	1.310259	0.873237	**H**	-6.740307	0.073628	-0.089497
H	-3.65101	5.73026	-0.782364	**H**	-5.90338	-0.399719	0.023072	**H**	-3.531725	-5.457944	-0.171972
H	-1.191418	5.83863	-0.724894	**C**	-4.718863	3.17031	0.852705	**H**	-1.113706	-5.585915	-0.153603
H	0.826862	5.58496	-1.463953	**H**	-5.601788	3.733135	1.139603	**H**	1.111483	-5.586288	-0.153492
H	3.253967	5.555326	-1.500317	**C**	4.985573	2.761843	-0.812423	**H**	3.529769	-5.459149	-0.170527
H	4.483431	3.55029	-0.900594	**H**	5.926718	3.227195	-1.090729	**H**	6.740446	0.071609	-0.091171
H	5.518304	2.173696	0.402975	**C**	0.206221	5.857064	-0.291321	**H**	5.684866	-2.771457	1.41655
H	6.769394	0.043283	0.495448	**H**	0.235364	6.939774	-0.376855	**H**	-5.686424	-2.766862	1.419534
H	5.54559	-2.102896	0.40304	**C**	-0.115498	-5.399332	-0.892651	**C**	-5.017014	1.382207	-0.044172
H	4.528706	-3.493319	-0.899303	**H**	-0.120413	-6.436956	-1.21232	**C**	-3.566846	4.041147	-0.017302
H	3.325254	-5.514516	-1.497374	**S**	-5.30424	-2.643275	-0.160554	**H**	-4.651188	4.065315	-0.022481
S	1.320935	2.707912	0.820986	**S**	4.957795	-2.927891	1.225598	**H**	-5.655762	2.257993	-0.072956
S	1.355358	-2.6907	0.821145					**S**	-5.281244	-2.804337	0.056985
C	-2.989085	-0.019035	0.124448					**S**	5.280377	-2.805713	0.055878

Table S6 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states. The values were obtained using B3LYP/6-31G* for the optimized ground state geometry. Water was taken into account as a 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

Table S7 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-N2.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-N2	1	0.27	4559.16	0.0054
	2	0.69	1789.30	0.0258
	3	0.84	1479.22	0.0573
	4	1.30	948.82	0.1754
	5	1.65	753.04	0.0103
	6	1.82	681.50	0.0013
	7	2.01	617.87	0.0552
	8	2.38	520.74	0.1736
	9	2.77	447.50	0.0839
	10	2.96	418.90	0.1054
	11	3.11	399.09	0.0752
	12	3.28	377.91	0.1016
	13	3.30	375.19	0.0043
	14	3.33	372.13	0.0588
	15	3.39	365.36	0.1286
	16	3.45	359.72	0.2155
	17	3.45	359.29	0.2304
	18	3.63	341.85	0.0006
	19	3.74	331.17	0.0310
	20	3.83	323.39	0.0909

Table S8 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-N2-*h*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-N2-*h*	1	2.89	428.87	0.0070
	2	3.01	411.92	0.0006
	3	3.32	373.70	0.1899
	4	3.33	372.72	0.1253
	5	3.41	363.43	0.7655
	6	3.43	361.85	0.7799
	7	3.56	348.08	0.0013
	8	3.58	345.92	0.0146
	9	3.86	321.44	0.0001
	10	3.93	315.85	0.0083
	11	3.95	314.01	0.0117
	12	4.14	299.73	0.0058
	13	4.18	296.37	0.0029
	14	4.22	294.05	0.0023
	15	5.24	291.69	0.0005
	16	4.28	289.89	0.0004
	17	4.30	288.46	0.0000
	18	4.31	287.61	0.0068
	19	4.31	287.45	0.0295
	20	4.35	285.23	0.0085

Table S9 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-N2-*p*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-N2-*p*	1	2.76	449.85	0.0023
	2	2.79	444.54	0.1089
	3	3.26	380.86	0.6370
	4	3.26	380.79	0.9164
	5	3.37	367.40	0.0728
	6	3.57	347.08	0.0280
	7	3.61	343.60	0.0753
	8	3.72	333.30	0.0115
	9	3.79	326.95	0.0745
	10	3.83	323.39	0.0603
	11	3.96	312.99	0.0001
	12	3.97	312.25	0.0568
	13	4.07	304.66	0.0007
	14	4.10	303.01	0.0344
	15	4.16	297.74	0.0056
	16	4.23	293.02	0.0233
	17	4.24	292.62	0.0464
	18	4.28	289.58	0.0383
	19	4.30	288.66	0.0654
	20	4.34	285.50	0.0054

Table S10 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-B2.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-B2	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
	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

Table S11 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-B2-*h*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-B2-*h*	1	2.82	439.04	0.0421
	2	2.90	428.16	0.0000
	3	2.93	423.11	0.0029
	4	2.93	422.49	0.0024
	5	3.08	403.17	0.0059
	6	3.09	401.15	0.0000
	7	3.12	397.83	0.0000
	8	3.16	392.01	0.0631
	9	3.30	375.34	0.8771
	10	3.33	372.27	0.7529
	11	3.56	347.86	0.0042
	12	3.64	340.23	0.0013
	13	3.67	338.13	0.0000
	14	3.71	333.81	0.0002
	15	3.75	330.52	0.0001
	16	3.85	321.98	0.0115
	17	3.92	316.21	0.0023
	18	3.94	315.01	0.0052
	19	3.95	314.22	0.0000
	20	3.98	311.39	0.0104

Table S12 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-B2-*p*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-B2-*p*	1	1.95	635.71	0.0002
	2	2.08	596.84	0.0070
	3	2.33	531.67	0.0153
	4	2.49	497.67	0.0171
	5	2.56	484.53	0.1902
	6	2.79	443.83	0.0538
	7	3.19	389.20	0.2709
	8	3.25	381.85	0.0824
	9	3.29	376.69	0.0001
	10	3.41	363.68	0.0014
	11	3.46	358.28	0.0000
	12	3.49	355.63	0.0775
	13	3.50	354.57	0.0030
	14	3.65	340.03	0.4067
	15	3.69	336.10	0.0027
	16	3.73	332.13	0.4369
	17	3.79	327.52	0.0015
	18	3.81	325.43	0.0020
	19	3.83	323.55	0.0842
	20	3.84	322.63	0.6276

Table S13 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-P2.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-P2	1	0.34	3697.24	0.0288
	2	1.41	881.49	0.0079
	3	1.43	867.11	0.0016
	4	1.63	759.29	0.0274
	5	1.84	672.12	0.0312
	6	1.87	664.77	0.0090
	7	2.21	562.06	0.0068
	8	2.28	542.91	0.0207
	9	2.40	515.80	0.1793
	10	2.72	455.79	0.0151
	11	2.89	429.05	0.0021
	12	3.09	401.33	0.0048
	13	3.14	395.10	0.0048
	14	3.16	392.74	0.0078
	15	3.16	392.30	0.0100
	16	3.23	384.21	0.0026
	17	3.30	376.54	0.0052
	18	3.48	355.90	0.0434
	19	3.51	352.93	0.0551
	20	3.54	350.65	0.0980

Table S14 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-P2-*h*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-P2-*h*	1	2.73	453.90	0.0010
	2	2.83	438.81	0.0521
	3	3.16	391.82	0.1902
	4	3.17	391.41	0.7924
	5	3.21	385.77	0.5377
	6	3.26	380.31	0.0888
	7	3.42	362.48	0.0488
	8	3.48	356.07	0.0797
	9	3.56	348.41	0.0298
	10	3.59	345.32	0.1504
	11	3.81	325.25	0.0074
	12	3.89	318.90	0.0195
	13	3.91	317.39	0.0162
	14	3.99	310.92	0.0204
	15	4.02	308.37	0.0423
	16	4.08	303.63	0.0315
	17	4.13	300.56	0.0434
	18	4.15	298.68	0.0006
	19	4.20	294.71	0.0030
	20	4.22	293.47	0.0257

Table S15 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-P2-*p*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-P2-*p*	1	2.48	499.13	0.1840
	2	2.57	483.25	0.0479
	3	2.99	414.49	0.5699
	4	3.05	406.38	0.3999
	5	3.08	403.17	0.0445
	6	3.42	362.15	0.0684
	7	3.47	357.73	0.0150
	8	3.47	357.35	0.0504
	9	3.51	353.44	0.0147
	10	3.61	343.51	0.0605
	11	3.72	333.64	0.1679
	12	3.73	332.58	0.1707
	13	3.76	330.18	0.0031
	14	3.80	326.29	0.4717
	15	3.86	321.46	0.0001
	16	3.87	320.03	0.0433
	17	3.88	319.18	0.1448
	18	4.01	309.17	0.0535
	19	4.10	301.98	0.1140
	20	4.14	299.05	0.0522

Table S16 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-S2.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-S2	1	1.47	844.13	0.0297
	2	1.63	760.03	0.0213
	3	1.68	738.80	0.0204
	4	1.77	699.56	0.0192
	5	2.12	583.80	0.1320
	6	2.16	572.69	0.0547
	7	2.47	501.53	0.0026
	8	2.62	473.47	0.0270
	9	2.64	470.34	0.0082
	10	2.73	454.10	0.0002
	11	2.96	419.48	0.0028
	12	3.08	402.59	0.0080
	13	3.09	401.46	0.0353
	14	3.11	399.30	0.0000
	15	3.17	390.68	0.1011
	16	3.29	377.21	0.0350
	17	3.34	371.70	0.0344
	18	3.44	359.92	0.1676
	19	3.51	353.13	0.3884
	20	3.84	350.38	0.1874

Table S17 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-S2-*h*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-S2-*h*	1	0.12	10649.67	0.0017
	2	1.00	1245.55	0.0703
	3	1.33	931.98	0.0580
	4	1.72	719.56	0.0768
	5	2.10	592.90	0.0014
	6	2.21	562.27	0.0708
	7	2.28	544.26	0.1024
	8	2.50	495.48	0.0691
	9	2.59	478.20	0.4259
	10	2.63	470.59	0.0181
	11	2.78	446.70	0.0586
	12	2.98	416.52	0.0642
	13	3.07	403.05	0.0980
	14	3.20	387.89	0.0117
	15	3.29	376.77	0.0153
	16	3.39	365.86	0.0033
	17	3.46	358.03	0.0128
	18	3.48	356.21	0.1026
	19	3.5194	352.29	0.0176
	20	3.6009	344.32	0.1500

Table S18 Absorption energy, wavelengths, and oscillator strengths for the first 20 singlet states of C42-S2-*p*.

	Singlet states	Absorption energy (eV)	Wavelength (nm)	Oscillator strengths(f)
C42-S2-*p*	1	0.65	1893.77	0.0590
	2	0.71	1740.58	0.0036
	3	1.48	839.03	0.0204
	4	1.60	775.68	0.3044
	5	1.82	682.88	0.0334
	6	1.93	643.96	0.0139
	7	2.05	606.06	0.0071
	8	2.15	575.84	0.0269
	9	2.21	559.88	0.0737
	10	2.50	495.32	0.0385
	11	2.71	457.11	0.1080
	12	2.77	447.63	0.1286
	13	2.94	421.74	0.0437
	14	3.12	397.51	0.0101
	15	3.14	395.43	0.6457
	16	3.20	388.41	0.2987
	17	3.44	360.05	0.2484
	18	3.58	346.52	0.0003
	19	3.62	342.19	0.0301
	20	3.67	337.56	0.0171

Table S19 Excitation energies, wavelengths, oscillator strengths, transition coefficients, and associated eigenvalues of the prominent excitation in N- and S-doped GQDs.

GQDs	Dominant Excitation	Excitation energy(eV)	Wavelength (nm)	Oscillator strength(f)	Transition coefficients	Associated eigenvalues(λ_i)
C42-N2	S17	3.45	359.29	0.23	H-3→L+2 -0.29	0.62
					H-2→L+1 0.53	0.28
					H-1→L+2 -0.27	
C42-N2-*h*	S5	3.41	363.43	0.77	H-1→L+1 0.47	
					H→L 0.39	0.48
					H →L+2 0.30	0.48
	S6	3.43	361.85	0.78	H-2→L 0.29	
					H-1→L -0.38	0.57
					H-1→L+2 -0.28	0.36
					H→L+1 0.42	
C42-N2-*p*	S4	3.26	380.79	0.92	H-1→L 0.51	0.52
					H→L+1 -0.45	0.41
C42-S2	19	3.51	353.13	0.39	H-4→L 0.50	0.59
					H-2→L+1 -0.37	0.30
C42-S2-*h*	9	2.59	478.20	0.43	H →L+5 0.60	0.80
C42-S2-*p*	15	3.14	395.43	0.65	H-2→L -0.47	0.47
					H-1→L+1 0.49	0.46