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Electronic Supplementary Information

for

Revealing incorporation of NH_2 group into the edge of carbon dots for H_2O_2 sensing via C–N···H hydrogen bond interaction: A DFT and TDDFT study

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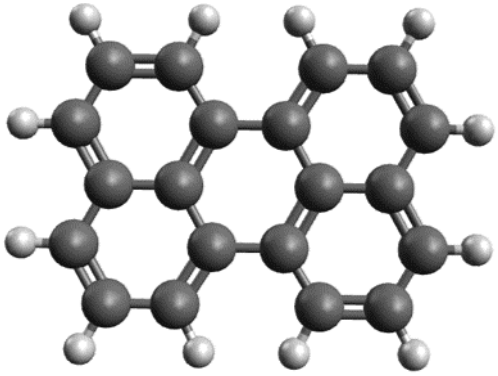

Fig. S1. Optimized molecular geometry for carbon dots without -NH_2 group

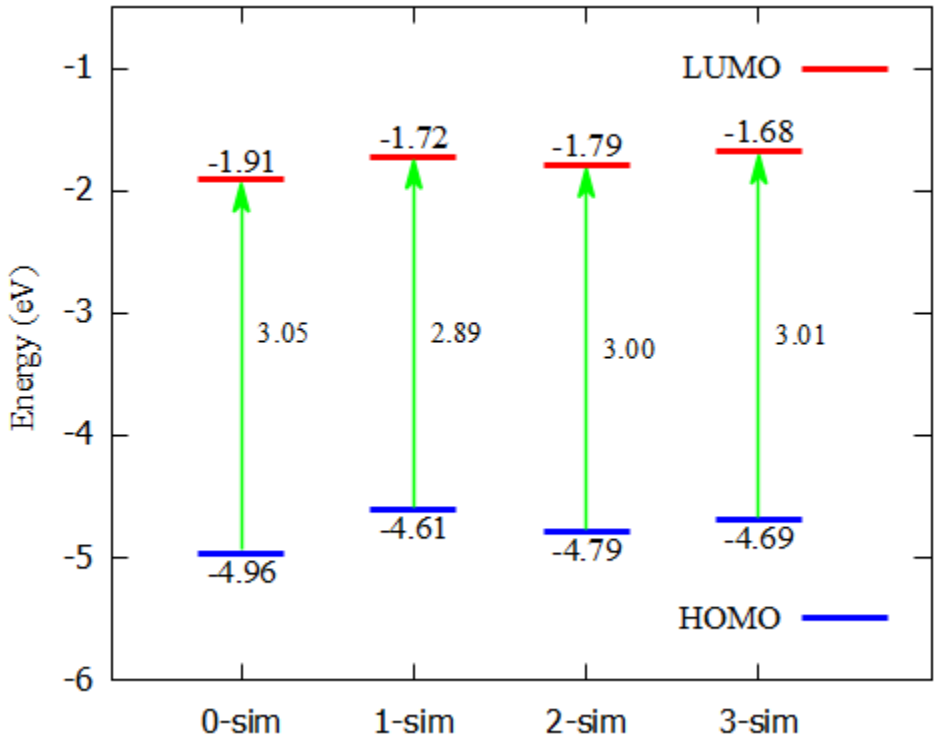

Fig. S2. Energy level diagram for carbon dots with and without -NH_2 group

Table S1

Mulliken atomic charge distribution for NH_2-carbon dots before and after interacts with H_2O_2.

Atomic	1-sim	1-com	Atomic	2-sim	2-com	Atomic	3-sim	3-com
C1	-0.09015	-0.09415	C1	-0.08792	-0.08793	C1	-0.09603	-0.09464
C2	-0.16312	-0.16174	C2	-0.16119	-0.1615	C2	-0.16012	-0.1592
C3	-0.15562	-0.15386	C3	-0.16693	-0.1647	C3	-0.15252	-0.15277
C4	0.061046	0.061853	C4	0.07477	0.072243	C4	0.051095	0.052998
C5	-0.08822	-0.0881	C5	-0.0883	-0.08828	C5	-0.08864	-0.08832
C6	-0.13691	-0.13573	C6	-0.13628	-0.13547	C6	-0.13675	-0.13596
C7	0.072485	0.072121	C7	0.072713	0.073642	C7	0.070366	0.070707
C8	0.017122	0.019707	C8	0.021389	0.02246	C8	0.014015	0.016197
C9	0.094103	0.093052	C9	0.091687	0.091114	C9	0.094959	0.094357
C10	-0.13958	-0.13733	C10	-0.13532	-0.13435	C10	-0.13825	-0.13654
C11	-0.08753	-0.0879	C11	-0.08907	-0.08976	C11	-0.08792	-0.08838
C12	-0.14206	-0.1433	C12	-0.14077	-0.14031	C12	-0.13389	-0.13349
C13	0.080652	0.088036	C13	0.095709	0.092062	C13	0.098049	0.101603
C14	0.012037	0.012377	C14	0.017213	0.025041	C14	0.008353	0.005325
C15	0.074283	0.081089	C15	0.07137	0.065473	C15	0.058865	0.068083
C16	0.077001	0.074753	C16	0.068842	0.066273	C16	0.074032	0.074101
C17	-0.16569	-0.16361	C17	-0.15904	-0.16153	C17	-0.21415	-0.21073
C18	0.226557	0.206843	C18	-0.18362	-0.17761	C18	-0.14452	-0.14644
C19	-0.11686	-0.11205	C19	0.292126	0.267422	C19	-0.09855	-0.1049
C20	-0.17107	-0.17447	C20	-0.18815	-0.19628	C20	0.191993	0.171314
H1	0.082316	0.085179	H1	0.084558	0.087546	H1	0.082302	0.084768
H2	0.079114	0.081366	H2	0.080997	0.099912	H2	0.118116	0.108798
H3	0.08346	0.086602	H3	0.073187	0.115675	N	-0.66954	-0.71467
H4	0.07152	0.077647	N	-0.66367	-0.70747	H3	0.078262	0.111966
N	-0.66478	-0.70832	H4	0.068376	0.069793	H4	0.086345	0.090642
H5	0.080655	0.077755	H5	0.077718	0.078519	H5	0.080552	0.0835
H6	0.084009	0.084104	H6	0.082225	0.083777	H6	0.08275	0.084876
H7	0.08391	0.085282	H7	0.079904	0.081656	H7	0.083497	0.084777
H8	0.081474	0.0834	H8	0.084049	0.083857	H8	0.082875	0.084655
H9	0.083476	0.085945	H9	0.085081	0.085276	H9	0.083483	0.08549
H10	0.081464	0.08386	H10	0.082428	0.083168	H10	0.080635	0.08253

H11	0.079655	0.082636	H11	0.082922	0.083223	H11	0.080314	0.082835
H12	0.258033	0.291861	H12	0.25701	0.260496	H12	0.263265	0.265838
H13	0.257222	0.26895	H13	0.255971	0.285327	H13	0.256769	0.285074
O1	-	-0.37118	O1	-	-0.36534	O1	-	-0.36189
O2	-	-0.35153	O2	-	-0.35901	O2	-	-0.35499
H14	-	0.359815	H14	-	0.358668	H14	-	0.353892
H15	-	0.339028	H15	-	0.336885	H15	-	0.338583

Table S2

Wavelength (λ) and oscillator strength (f) in UV-Vis absorption characteristics.

1-sim		2-sim		3-sim		1-com		2-com		3-com	
λ (nm)	f	λ (nm)	f	λ (nm)	f	λ (nm)	f	λ (nm)	f	λ (nm)	f
394.71	0.4729	380.99	0.4046	386.52	0.3795	388.81	0.5089	375.93	0.4266	378.94	0.4007
309.01	0.0050	318.61	0.0415	303.42	0.0146	306.08	0.0031	307.79	0.0139	300.86	0.0128
284.12	0.0018	289.99	0.0108	292.16	0.0152	283.15	0.0001	287.41	0.0155	290.27	0.0122
279.59	0.0040	272.48	0.0021	276.76	0.0023	276.92	0.0032	272.81	0.0006	274.76	0.0005
266.97	0.0283	257.14	0.0280	255.95	0.0192	261.82	0.0089	254.25	0.0265	252.73	0.0149
250.48	0.0201	249.52	0.0024	251.36	0.0739	249.95	0.0150	249.00	0.0014	249.54	0.0848
247.38	0.0030	242.51	0.0017	249.47	0.0121	245.88	0.0011	241.58	0.0031	248.067	0.0059
237.47	0.0058	236.24	0.0078	237.74	0.0041	238.31	0.0025	236.17	0.0030	237.83	0.0056
223.16	0.7011	220.42	0.7304	226.13	0.6565	221.25	0.7265	219.42	0.8130	225.35	0.7348
212.15	0.000	217.78	0.0597	214.69	0.1295	210.08	0.0006	212.67	0.0968	212.60	0.0970

Table S3

Charge transfer length (Δr) in Angstrom (Å) calculated by TDDFT.

Excited states	1-sim	1-com	2-sim	2-com	3-sim	3-com
1	0.6621	0.4650	0.7636	0.4074	0.4395	0.3138
2	0.6769	0.7320	1.9537	1.6397	1.0786	1.1680
3	1.1203	1.1890	1.5226	1.2697	1.2383	1.2558
4	0.8669	0.8300	0.9065	0.7367	0.7388	0.7029
5	0.7885	0.7198	1.0214	0.7860	0.6287	0.7460
6	0.8206	0.6751	0.8196	0.6548	0.8576	0.6874
7	0.7183	0.6638	0.7880	0.6822	0.7188	0.6803
8	0.4099	0.4164	0.9517	0.7812	0.4767	0.3868
9	1.0876	1.1657	1.1077	0.9936	1.1078	0.9961
10	0.7102	0.8159	1.8717	1.8569	1.5855	1.6967