

Supplementary Information: Tuning functionalized hexagonal boron nitride quantum dots for full visible-light fluorescence emission

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1. Localized orbital locator (LOL) function

Localized orbital locator (LOL) function is defined as follows:¹

$$LOL(r) = \frac{\tau(r)}{1 + \tau(r)} \quad (1)$$

in which

$$\tau(r) = \frac{D_0(r)}{\left(\frac{1}{2}\right) \sum_i \eta_i |\nabla \varphi_i|^2} \quad (2)$$

where $D_0(r)$ is the exact kinetic energy density of non-interacting, uniform electron gas.

$LOL(r)$ is the ratio of the kinetic energy density of uniform electron gas to kinetic energy density of real system. Relatively lower kinetic energy density of real system compared to the kinetic energy density of uniform electron gas means large $LOL(r)$ and high orbital localization.

2. Quantitative characterization of the electron–hole distribution in the whole space²

To evaluate overlapping extent of electron and hole, S_r index is defined as follows:

$$S_r \text{ index} = \int S_r(r) dr \equiv \int \sqrt{\rho^{hole}(r)\rho^{ele}(r)} dr \quad (3)$$

The most representative position of electron–hole distribution is obtained via calculating centroid. For example, X coordinate of electron centroid is expressed as

$$X_{ele} = \int x \rho^{ele}(r) dr \quad (4)$$

in which x is X component of position vector r .

The charge transfer (CT) length in X/Y/Z can be measured by distance between centroid of electron and hole in corresponding directions:

$$D_x = |X_{ele} - X_{hole}| \quad (5)$$

$$D_y = |Y_{ele} - Y_{hole}| \quad (6)$$

$$D_z = |Z_{ele} - Z_{hole}| \quad (7)$$

The total magnitude of CT length is referred to as D index:

$$D \text{ index} = |D| \equiv \sqrt{(D_x)^2 + (D_y)^2 + (D_z)^2} \quad (8)$$

The RMSD of electron and hole can be used to characterize their extent of spatial distribution. For example, X component of RMSD of hole is expressed as

$$\sigma_{hole,x} = \sqrt{\int (x - X_{hole})^2 \rho^{hole}(r) dr} \quad (9)$$

The $|\sigma_{hole}|$ and $|\sigma_{ele}|$ refer to σ_{hole} and σ_{ele} indices and they measure overall RMSD of electron and hole, respectively.

H index is overall average degree of spatial extension of electron–hole distribution.

$$H \text{ index} = (|\sigma_{ele}| + |\sigma_{hole}|)/2 \quad (10)$$

t index is designed to measure separation degree of electron and hole in CT direction:

$$t \text{ index} = D \text{ index} - H_{CT} \quad (11)$$

H_{CT} is average degree of spatial extension of electron and hole in CT direction. To calculate H_{CT} , the following relationship is defined:

$$H_{CT} = |H \cdot u_{CT}| \quad (12)$$

where u_{CT} is unit vector in CT direction and can be straightforwardly derived using centroid of electron and hole.

If t index < 0, it implies that electron hole and is not substantially separated due to CT.

3. Orbital hybridization³

Based on the chemical bonding theory, supposing that one system contains two atoms (A and B). The A atom has one orbital φ_A and its orbital energy is ε_A ; and the B atom has one orbital φ_B and corresponding orbital energy is ε_B . The molecular orbital can be expressed as the linear combination of φ_A and φ_B

$$\varphi = c[\varphi_A + \lambda\varphi_B] \quad (13)$$

in which c is the normalization coefficient and λ is expansion coefficient.

If $\lambda \rightarrow 0$ or $\lambda \rightarrow \infty$, φ is entirely composed by either φ_A or φ_B , thereto no hybridization. If $\lambda = 1$ means the full hybridization.

References

1. H.L. Schmider and A.D. Becke, *J. Mol. Struct.–THEOCHEM*, **2000**, 527, 51.
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3. X. Niu, Y. Li, H. Shu and J. Wang, *Nanoscale*, **2016**, 8, 19376.

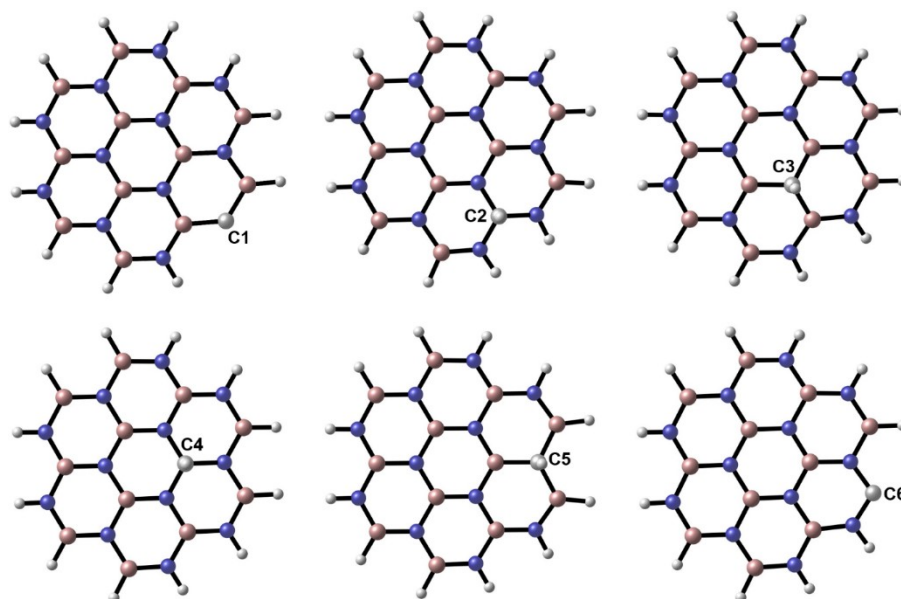


Figure S1. B3LYP-D3BJ/6-31G** optimized ground state structures of single sp^2 -C or sp^3 -C atom doped BNQDs.

Table S1. B3LYP-D3BJ/6-31G** Calculated Vertical Emission Energies (E_{\perp} /eV), Oscillator Strengths (f), Wavelength (λ /nm), Key Electronic Configurations, and State Assignments Based on the S_1 Minima of Single sp^3 -C Atom Doped BNQDs.

	E_{\perp} (eV)	λ (nm)	f	Configuration s	note
C1	–	–	–	–	Ground state is T_1 .
C2	4.59	270	0.0015	H–L (97.9 %)	
C3	4.83	257	0.0090	H–L (97.2 %)	
C4	3.21	386	0.0123	H–L (98.8 %)	
C5	1.75	707	0.0192	H–L (99.1 %)	
C6	2.14	579	0.0013	H–L (94.5 %)	Ground state is S_0 .

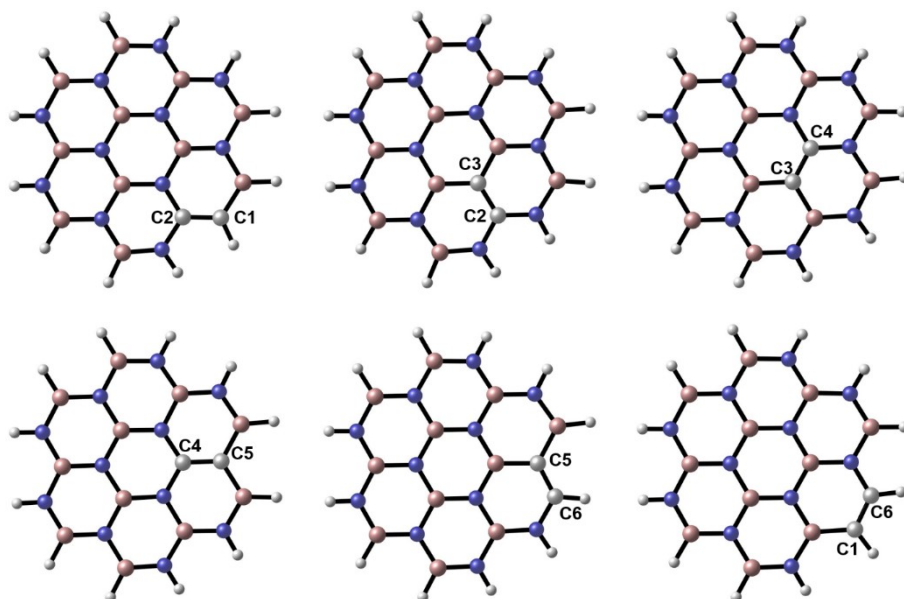


Figure S2. B3LYP-D3BJ/6-31G** optimized ground state structures of C=C (sp^2 -C) doped BNQDs.

Table S2. B3LYP-D3BJ/6-31G** Calculated Vertical Emission Energies (E_{\perp} /eV), Oscillator Strengths (f), Wavelength (λ /nm), Key Electronic Configurations, and State Assignments Based on the S_1 Minima of C=C (sp^2 -C) Doped BNQDs.

	E_{\perp} (eV)	λ (nm)	f	Configurations
C1C2	3.93	315	0.1534	H-L (89.6 %)
C2C3	4.19	296	0.1277	H-L (97.5 %)
C3C4	4.94	315	0.0314	H-L (88.7 %)
C4C5	4.43	280	0.2791	H-L (95.5 %)
C5C6	4.46	266	0.2648	H-L (95.0 %)
C6C1	4.66	258	0.0069	H-L (93.9 %)

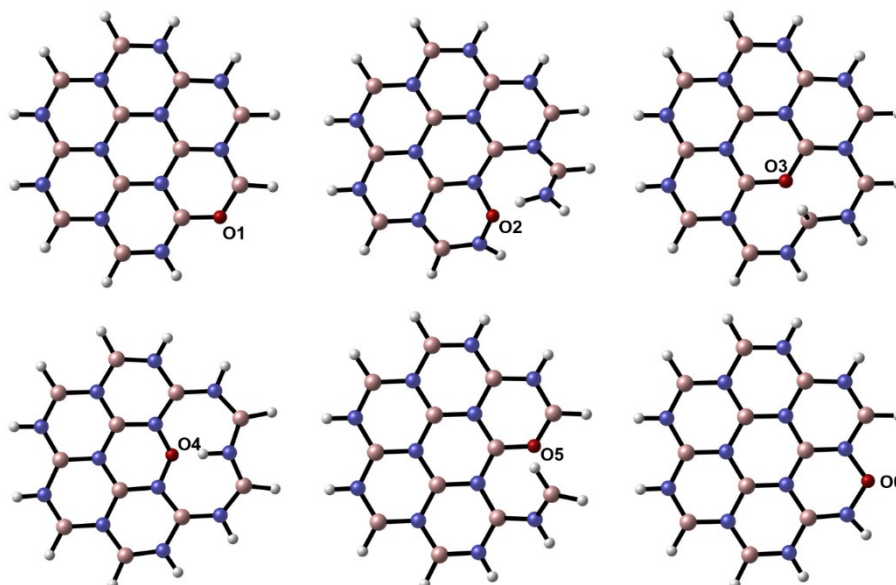


Figure S3. B3LYP-D3BJ/6-31G** optimized ground state structures of single O atom doped BNQDs.

Table S3. B3LYP-D3BJ/6-31G** Calculated Vertical Emission Energies (E_{\perp} /eV), Oscillator Strengths (f), Wavelength (λ /nm), Key Electronic Configurations, and State Assignments Based on the S_1 Minima of Single O Atom Doped BNQDs.

	E_{\perp} (eV)	λ (nm)	f	Configurations
O1	5.88	211	0.0403	H-L (44.1 %)
O2^b	-	-	-	-
O3	1.02	1217	0.0009	H-L (99.8 %)
O4	3.31	375	0.0079	H-L (99.6 %)
O5	1.98	625	0.0002	H-L (95.0 %)
O6	3.47	357	0.0024	H-L (97.7 %)

^b: No stable excited state structure was obtained in geometric optimization.

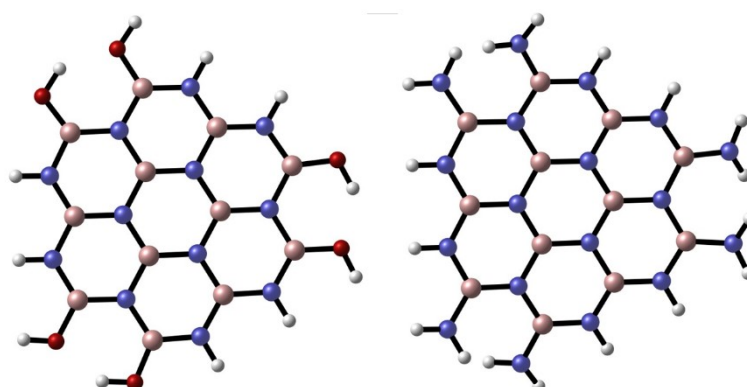


Figure S4. B3LYP-D3BJ/6-31G** optimized ground state structures of edge -OH and -NH₂ functionalized BNQDs.

Table S4. Calculated Vertical Emission Energies (E_{\perp} /eV), Oscillator Strengths (f), Wavelength (λ /nm), Key Electronic Configurations, and State Assignments Based on the S_1 Minima of edge -OH and -NH₂ functionalized BNQDs.

	E_{\perp} (eV)	λ (nm)	f	Configurations
OH ^a	6.69	185	0.2223	H→L (27.2 %), H-1→L+1 (27.8 %)
OH ^b	5.51	225	0.0008	
NH ₂ ^a	6.45	192	0.0003	H→L (44.7 %), H-1→L+1 (46.2 %)

^a: B3LYP-D3BJ/6-31G**

^b: B3LYP-D3BJ/6-311++G**//B3LYP-D3BJ/6-31G**

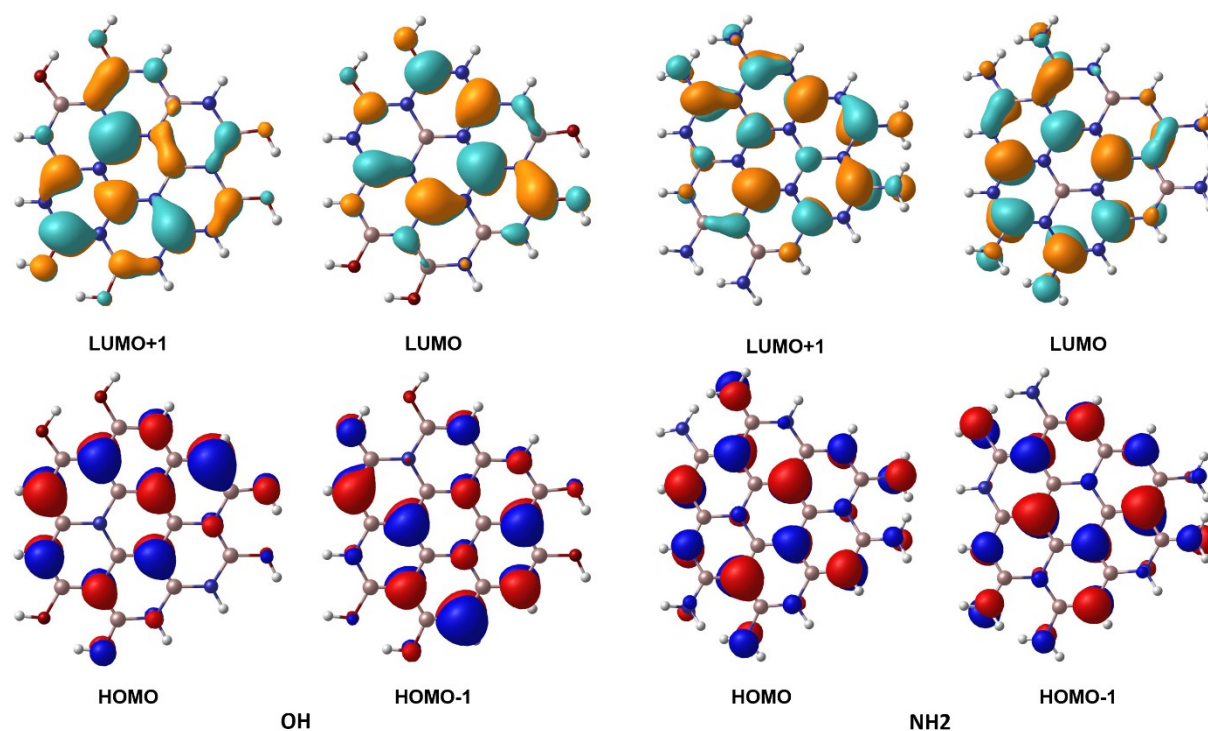


Figure S5. The frontier molecular orbitals at S_1 minima of edge -OH and -NH₂ functionalized BNQDs.

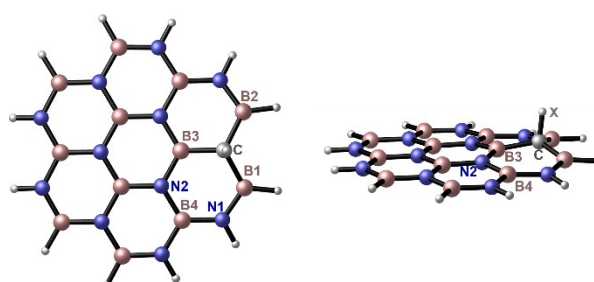


Figure S6 Top view (left) and side view (right) of optimized ground state structure of **d**. Also show atomic number.

Table S5. Selected Bond Length (in Å) and Dihedral Angle (in °) of BNQDs **a-f** at S_0 and S_1 Minima.

Bond Length (Å)	S_0			S_1		
	B1-C	B2-C	B3-C	B1-C	B2-C	B3-C
a	1.580	1.586	1.589	1.587	1.590	1.692
b	1.575	1.575	1.589	1.644	1.644	1.584
c	1.584	1.580	1.592	1.668	1.556	1.565
d	1.568	1.568	1.573	1.681	1.681	1.569
e	1.574	1.571	1.581	1.630	1.630	1.591
f	1.566	1.576	1.556	1.544	1.657	1.585
Dihedral Angle (°)	B4-N2-B3-C	B4-N1-B1-C	N2-B3-C-X	B4-N2-B3-C	B4-N1-B1-C	N2-B3-C-X
a	-12.0	-0.9	-80.5	-20.6	4.3	-85.8
b	-9.7	0.1	-90.2	-21.7	12.5	-91.7
c	-14.3	10.4	-81.4	-15.3	-6.8	-57.1
d	-10.0	2.0	-90.0	-25.1	16.5	-93.6
e	-10.3	-3.1	-96.2	-25.2	8.6	-91.0
f	-11.1	2.1	-94.1	-3.5	11.5	-107.2

X: the atom of substitute group directly connected with inserted sp^3 -C atom.

Table S6. B3LYP-D3BJ/6-311++G**/SMD Calculated Vertical Excitation Energies (E_{\perp} /eV), Oscillator Strengths (f), Wavelength (λ /nm) and Key Electronic Configurations of **a-f** in Aqueous Solution.

	States	E_{\perp} (eV)	f	λ (nm)	Configurations (NTO)
a	$S_0 \rightarrow S_1$	4.02	0.0039	308	H→L (99.86%)
	$S_0 \rightarrow S_2$	4.89	0.0045	253	H→L (98.99%)
	$S_0 \rightarrow S_4$	5.36	0.1630	231	H→L (98.15%)
	$S_0 \rightarrow S_9$	5.89	0.0553	211	H→L (91.10%)
b	$S_0 \rightarrow S_1$	4.47	0.0035	277	H→L (99.75%)
	$S_0 \rightarrow S_2$	4.81	0.0122	258	H→L (99.53%)
	$S_0 \rightarrow S_4$	5.35	0.1529	232	H→L (98.48%)
	$S_0 \rightarrow S_9$	5.86	0.0657	212	H→L (92.97%)
c	$S_0 \rightarrow S_1$	4.33	0.0032	286	H→L (99.84%)
	$S_0 \rightarrow S_2$	5.05	0.0244	246	H→L (99.55%)
	$S_0 \rightarrow S_4$	5.45	0.0335	228	H→L (74.60%)
	$S_0 \rightarrow S_9$	5.87	0.1982	211	H→L (85.09%)
d	$S_0 \rightarrow S_1$	5.71	0.0601	217	H→L (91.06%)
	$S_0 \rightarrow S_2$	5.94	0.0288	209	H→L (94.89%)
	$S_0 \rightarrow S_4$	6.04	0.3146	205	H→L (74.50%)
	$S_0 \rightarrow S_9$	6.30	0.0226	197	H→L (43.76%)
e	$S_0 \rightarrow S_1$	4.26	0.0211	291	H→L (99.75%)
	$S_0 \rightarrow S_2$	5.23	0.0120	237	H→L (97.00%)
	$S_0 \rightarrow S_4$	5.67	0.2166	219	H→L (89.14%)
	$S_0 \rightarrow S_9$	5.76	0.0215	215	H→L (69.69%)
f	$S_0 \rightarrow S_1$	4.54	0.0258	273	H→L (99.28%)
	$S_0 \rightarrow S_2$	4.71	0.0325	263	H→L (99.78%)
	$S_0 \rightarrow S_4$	5.84	0.1361	212	H→L (91.02%)

	S₀→S₉	6.00	0.1879	207	H→L (76.96%)
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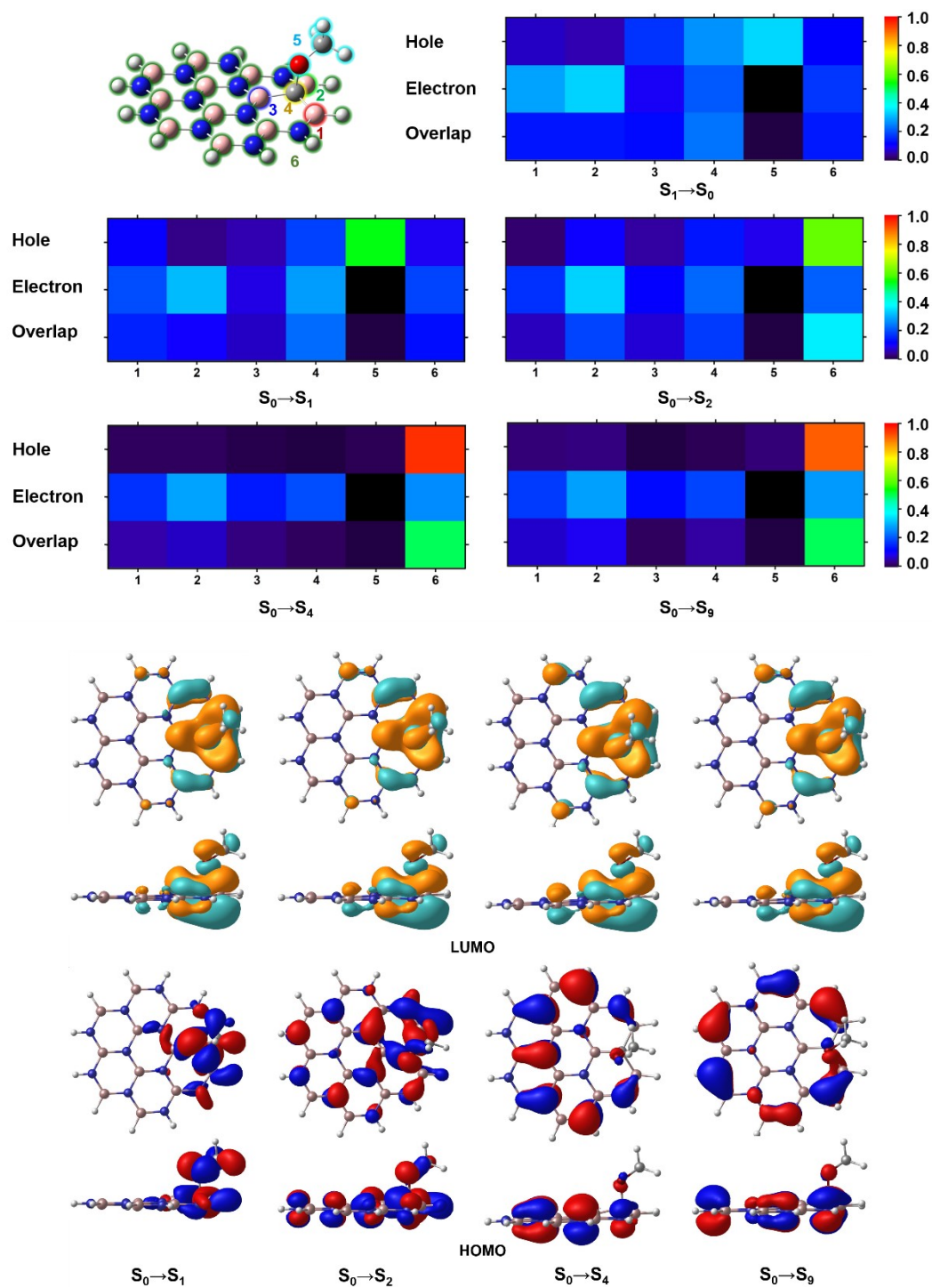


Figure S7. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for **a**.

Table S7. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for **a**.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
S₀→S₁	1	10.99	19.55	14.65	8.56
	2	3.32	30.86	10.12	27.54
	3	5.23	8.00	6.47	2.77
	4	18.24	27.85	22.54	9.61
	5	53.25	-4.90	0.00	-58.15
	6	8.97	18.64	12.93	9.67
S₀→S₂	1	2.25	16.52	6.09	14.27
	2	10.35	33.45	18.61	23.10
	3	4.66	11.30	7.26	6.64
	4	13.63	22.29	17.43	8.65
	5	8.52	-4.84	0.00	-13.36
	6	60.58	21.28	35.90	-39.30
S₀→S₄	1	1.56	16.33	5.04	14.77
	2	1.49	28.65	6.53	27.16
	3	0.58	13.97	2.86	13.38
	4	0.08	19.45	1.22	19.37
	5	0.96	-4.36	0.00	-5.32
	6	95.33	25.97	49.76	-69.36
S₀→S₉	1	2.61	17.51	6.76	14.89
	2	2.78	28.27	8.86	25.49
	3	0.17	12.44	1.44	12.27
	4	1.16	18.84	4.68	17.68
	5	2.55	-4.33	0.00	-6.88
	6	90.73	27.28	49.75	-63.45
S₁→S₀	1	6.34	28.60	13.47	22.26
	2	5.46	33.23	13.47	27.77
	3	16.69	9.37	12.51	-7.32
	4	26.48	20.50	23.30	-5.99
	5	33.60	-8.87	0.00	-42.47
	6	11.42	17.16	14.00	5.74

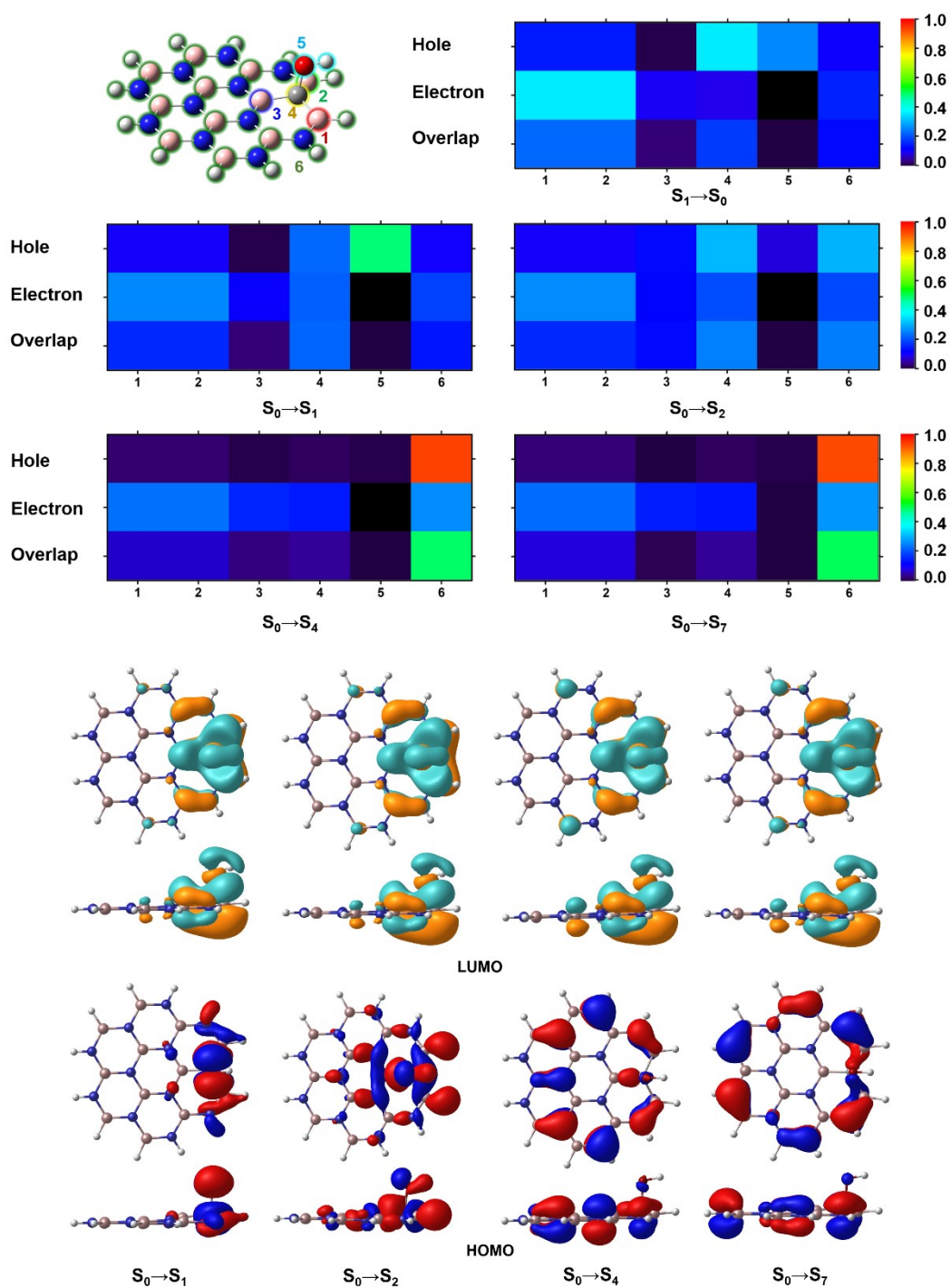


Figure S8. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for **b**.

Table S8. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for **b**.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
$S_0 \rightarrow S_1$	1	9.57	25.35	15.58	15.78
	2	9.52	25.36	15.54	15.84
	3	0.59	10.81	2.53	10.22
	4	22.18	21.65	21.91	-0.53
	5	48.27	-1.55	0.00	-49.82
	6	9.87	18.38	13.47	8.51
$S_0 \rightarrow S_2$	1	9.54	25.68	15.65	16.14
	2	9.60	25.69	15.71	16.09
	3	12.52	12.03	12.27	-0.49
	4	30.57	19.54	24.44	-11.03
	5	7.71	-2.21	0.00	-9.91
	6	30.06	19.27	24.07	-10.79
$S_0 \rightarrow S_4$	1	2.01	22.95	6.79	20.94
	2	2.00	22.96	6.78	20.96
	3	0.64	15.20	3.11	14.57
	4	1.22	13.90	4.12	12.68
	5	0.57	-0.68	0.00	-1.25
	6	93.56	25.66	49.00	-67.90
$S_0 \rightarrow S_7$	1	2.69	22.59	7.80	19.89
	2	2.70	22.60	7.81	19.90
	3	0.07	14.31	1.03	14.24
	4	1.33	13.57	4.24	12.24
	5	0.64	0.14	0.30	-0.49
	6	92.57	26.79	49.80	-65.78
$S_1 \rightarrow S_0$	1	13.82	35.67	22.21	21.85
	2	13.83	35.68	22.21	21.85
	3	0.69	9.19	2.51	8.50
	4	35.56	8.51	17.39	-27.05
	5	25.56	-3.62	0.00	-29.18
	6	10.55	14.58	12.40	4.03

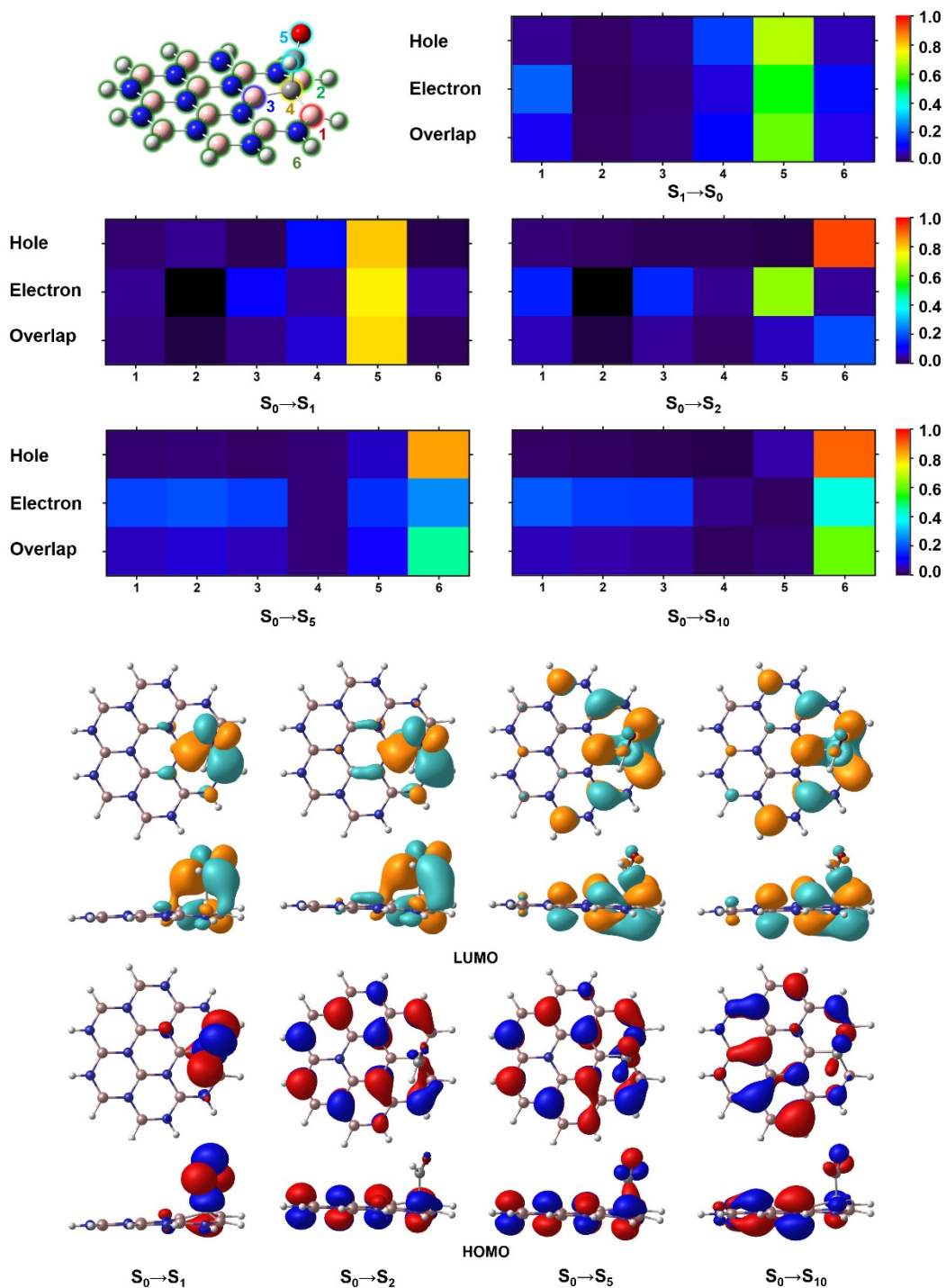


Figure S9. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for **c**.

Table S9. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for **c**.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
$S_0 \rightarrow S_1$	1	2.12	3.71	2.81	1.59
	2	3.55	-0.03	0.00	-3.58
	3	0.96	10.88	3.22	9.92
	4	12.51	4.20	7.25	-8.31
	5	80.38	76.51	78.42	-3.87
	6	0.49	4.73	1.53	4.24
$S_0 \rightarrow S_2$	1	2.43	14.22	5.88	11.79
	2	1.65	-2.00	0.00	-3.65
	3	1.14	15.23	4.17	14.09
	4	0.91	3.64	1.82	2.72
	5	0.58	64.80	6.13	64.23
	6	93.28	4.11	19.58	-89.17
$S_0 \rightarrow S_5$	1	2.10	18.37	6.22	16.26
	2	2.59	19.98	7.20	17.38
	3	1.79	17.44	5.58	15.65
	4	2.55	2.71	2.63	0.17
	5	6.36	15.75	10.01	9.39
	6	84.61	25.75	46.68	-58.86
$S_0 \rightarrow S_{10}$	1	1.58	20.69	5.72	19.11
	2	1.48	17.55	5.10	16.07
	3	0.96	17.16	4.06	16.19
	4	0.49	3.19	1.25	2.70
	5	5.05	1.25	2.52	-3.79
	6	90.43	40.16	60.27	-50.27
$S_1 \rightarrow S_0$	1	3.84	21.54	9.09	17.70
	2	1.74	1.52	1.63	-0.22
	3	3.29	2.59	2.92	-0.71
	4	17.85	7.61	11.65	-10.24
	5	67.73	54.25	60.62	-13.49
	6	5.55	12.50	8.33	6.94

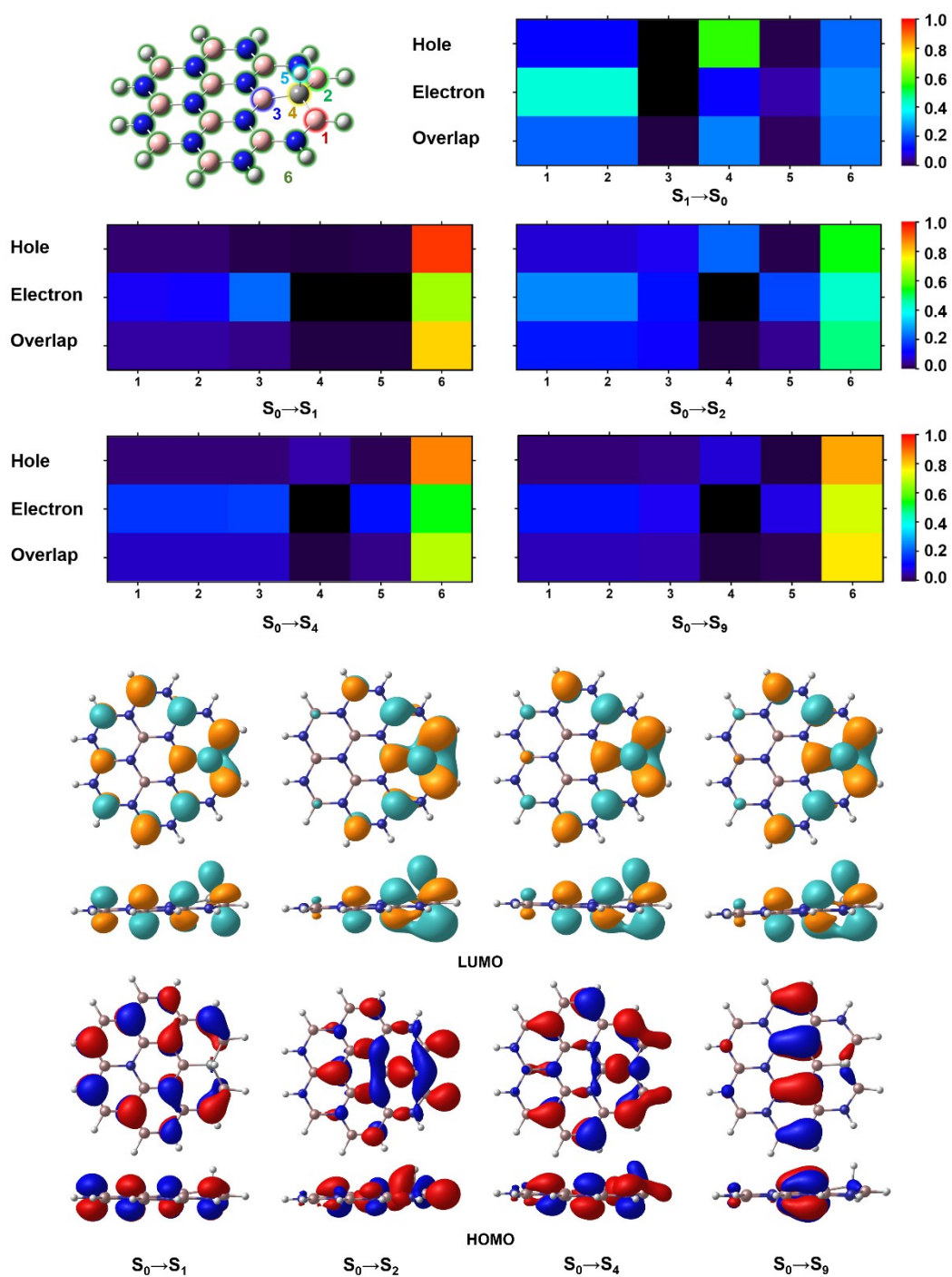


Figure S10. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for **d**.

Table S10. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for **d**.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
S₀→S₁	1	2.05	9.43	4.40	7.38
	2	2.05	10.06	4.54	8.00
	3	0.50	22.44	3.34	21.94
	4	0.00	-0.18	0.00	-0.19
	5	0.61	-19.05	0.00	-19.67
	6	94.66	66.31	79.23	-28.35
S₀→S₂	1	7.31	25.50	13.65	18.19
	2	7.32	25.44	13.64	18.12
	3	8.71	12.71	10.52	4.00
	4	22.03	-24.97	0.00	-47.00
	5	0.77	18.60	3.79	17.83
	6	53.86	42.73	47.97	-11.13
S₀→S₄	1	2.43	16.68	6.37	14.24
	2	2.43	16.71	6.37	14.27
	3	2.43	17.94	6.60	15.51
	4	4.83	-17.94	0.00	-22.77
	5	0.85	12.80	3.29	11.95
	6	87.03	53.82	68.44	-33.21
S₀→S₉	1	2.62	13.06	5.86	10.44
	2	2.63	13.15	5.88	10.53
	3	3.30	8.69	5.36	5.39
	4	7.15	-14.08	0.00	-21.23
	5	0.16	7.99	1.13	7.83
	6	84.13	71.18	77.38	-12.95
S₁→S₀	1	11.11	41.54	21.49	30.43
	2	11.12	41.56	21.50	30.44
	3	-0.93	-24.73	0.00	-23.80
	4	56.02	10.95	24.76	-45.07
	5	0.44	5.11	1.50	4.67
	6	22.24	25.57	23.85	3.34

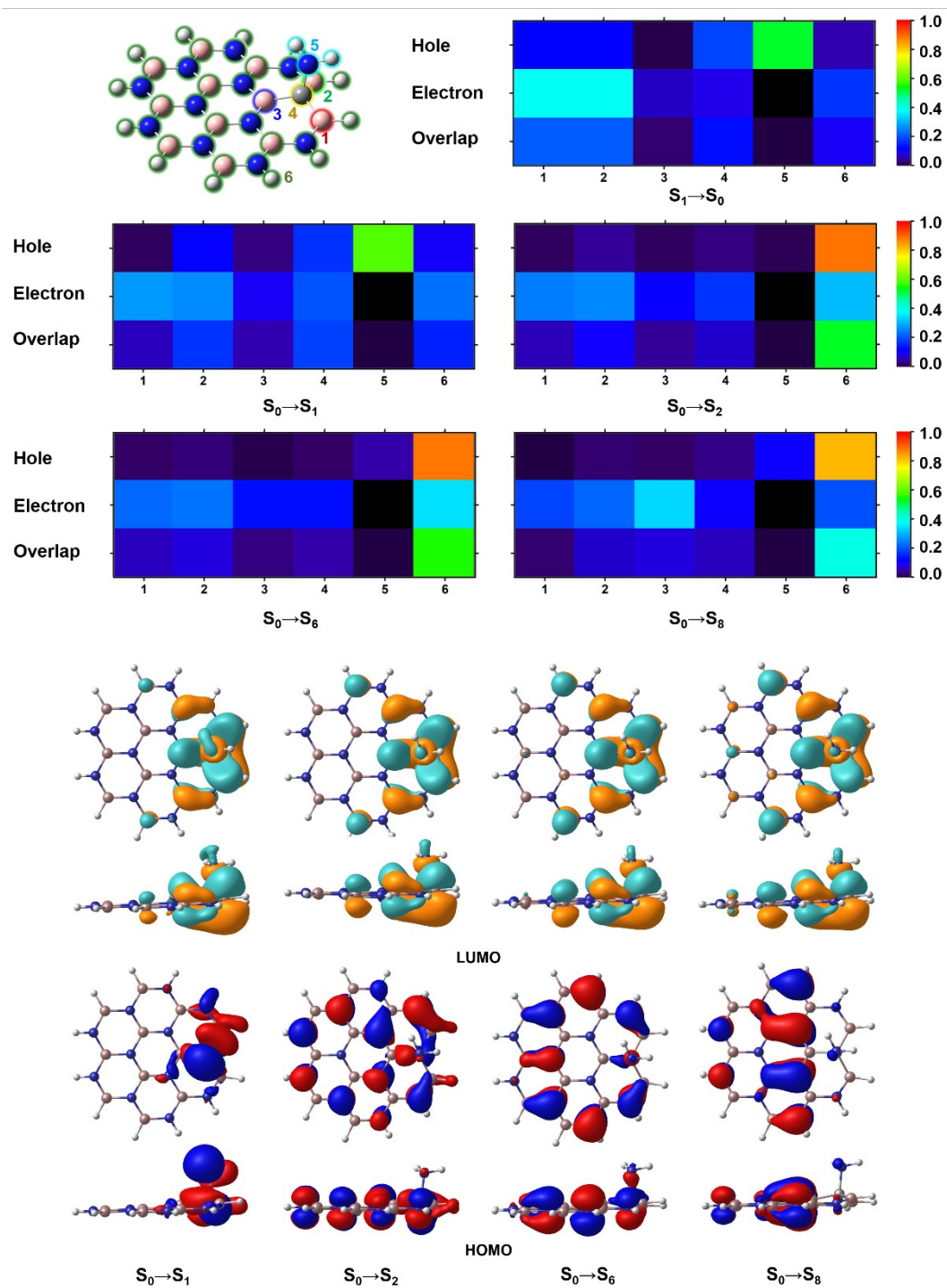


Figure S11. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for e .

Table S11. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for e.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
$S_0 \rightarrow S_1$	1	1.42	27.22	6.21	25.81
	2	11.03	25.62	16.81	14.60
	3	2.94	9.14	5.19	6.20
	4	16.45	20.14	18.20	3.69
	5	58.54	-5.17	0.00	-63.71
	6	9.63	23.05	14.90	13.42
$S_0 \rightarrow S_2$	1	1.43	24.17	5.89	22.73
	2	4.08	25.24	10.15	21.15
	3	1.57	10.86	4.13	9.29
	4	2.98	16.62	7.03	13.64
	5	1.02	-7.84	0.00	-8.86
	6	88.92	30.96	52.47	-57.96
$S_0 \rightarrow S_6$	1	1.77	22.07	6.24	20.30
	2	2.46	23.55	7.62	21.09
	3	0.74	12.78	3.08	12.04
	4	1.74	12.88	4.74	11.13
	5	4.77	-5.63	0.00	-10.40
	6	88.52	34.36	55.15	-54.15
$S_0 \rightarrow S_8$	1	0.24	18.77	2.10	18.54
	2	2.16	21.75	6.86	19.58
	3	1.73	33.75	7.64	32.03
	4	3.34	10.61	5.95	7.27
	5	10.49	-4.90	0.00	-15.40
	6	82.04	20.02	40.53	-62.02
$S_1 \rightarrow S_0$	1	11.44	38.94	21.11	27.49
	2	11.44	38.96	21.11	27.51
	3	0.76	6.56	2.23	5.81
	4	18.88	8.50	12.67	-10.38
	5	52.34	-9.68	0.00	-62.02
	6	5.14	16.72	9.27	11.58

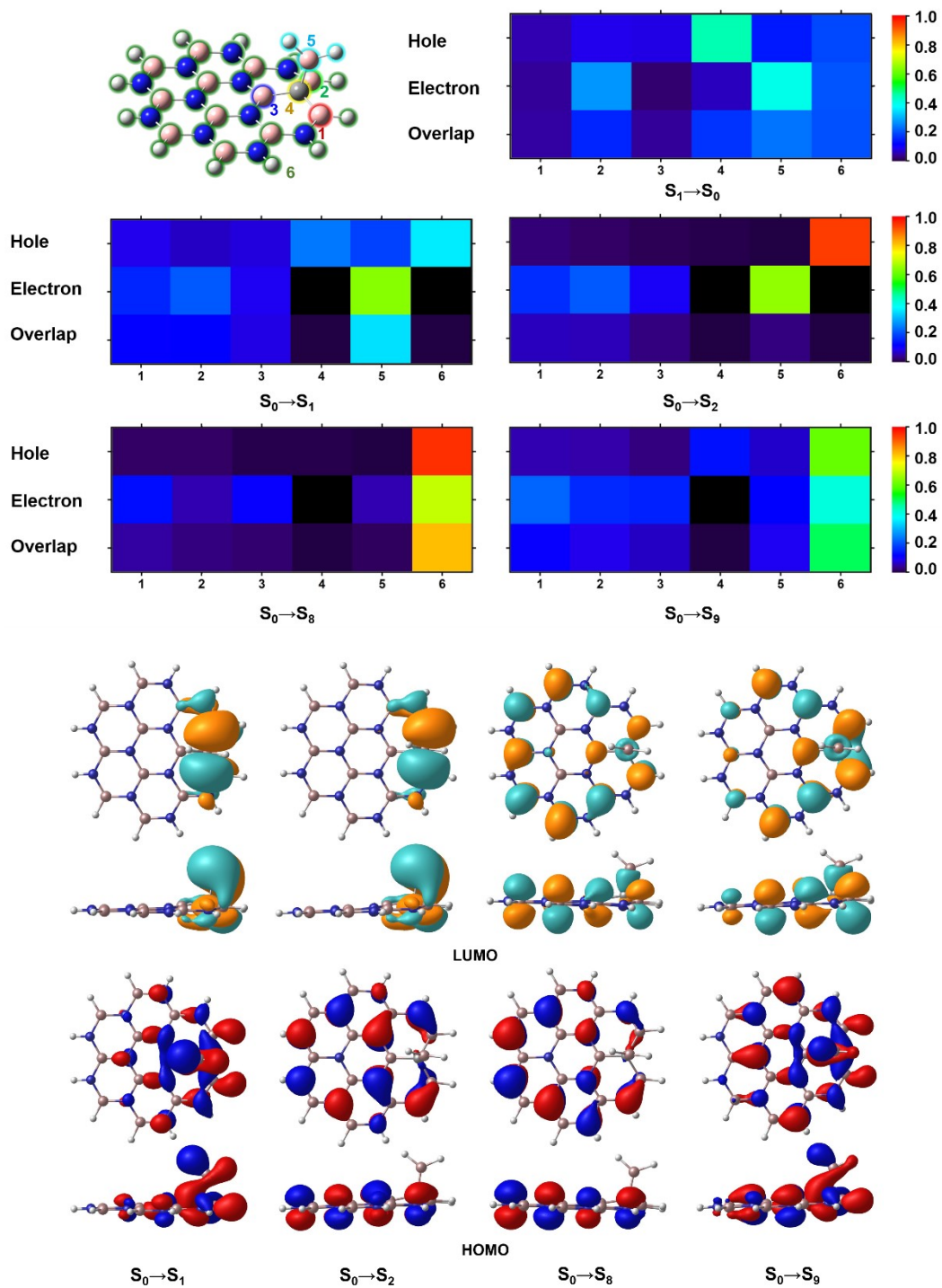


Figure S12. Electron–hole compositions in each fragment (top), and natural transition orbitals (NTO) in vertical excitation (down) for **f**.

Table S12. The Contribution (%) of Each Fragment to Electron and Hole in Vertical Excitation and Emission, also Collected the Overlap and Difference of Electron and Hole in Each Fragment for **f**.

	Fragment	Hole (%)	Electron (%)	Overlap (%)	Diff (%)
$S_0 \rightarrow S_1$	1	8.41	15.24	11.32	6.84
	2	6.42	20.49	11.47	14.08
	3	7.68	8.73	8.18	1.05
	4	23.69	-4.72	0.00	-28.41
	5	18.32	64.15	34.28	45.83
	6	35.49	-3.90	0.00	-39.39
$S_0 \rightarrow S_2$	1	2.48	15.90	6.28	13.42
	2	1.68	20.72	5.89	19.05
	3	0.96	9.27	2.98	8.31
	4	0.67	-7.21	0.00	-7.88
	5	0.15	64.90	3.14	64.75
	6	94.07	-3.57	0.00	-97.64
$S_0 \rightarrow S_8$	1	1.63	12.99	4.60	11.36
	2	1.59	5.40	2.93	3.81
	3	0.41	10.82	2.11	10.41
	4	0.75	-4.05	0.00	-4.80
	5	0.31	5.35	1.29	5.04
	6	95.31	69.49	81.38	-25.83
$S_0 \rightarrow S_9$	1	5.45	21.75	10.88	16.31
	2	4.84	15.38	8.62	10.54
	3	2.87	14.90	6.54	12.02
	4	13.04	-5.84	0.00	-18.88
	5	6.82	11.57	8.88	4.76
	6	60.41	40.96	49.75	-19.45
$S_1 \rightarrow S_0$	1	5.25	4.24	4.72	-1.00
	2	8.65	27.10	15.31	18.45
	3	8.04	2.20	4.20	-5.84
	4	45.14	6.16	16.67	-38.98
	5	13.97	39.84	23.59	25.87
	6	18.95	20.46	19.69	1.51

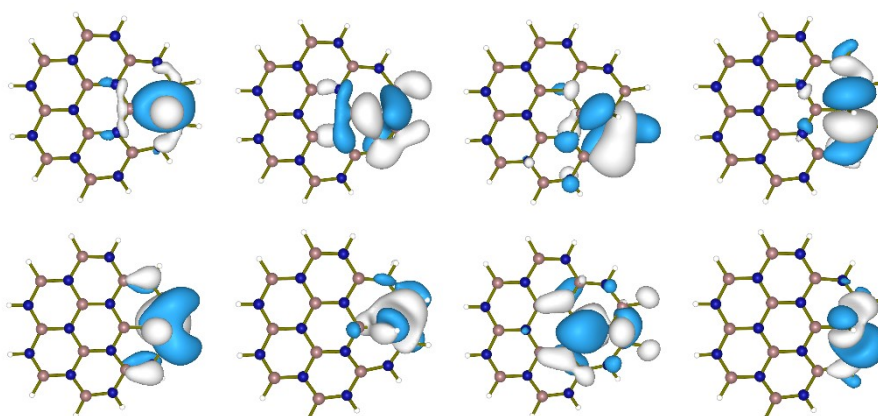


Figure S13. Molecular orbitals of **d** used in defining the active space for MS-CASPT2(8e/8o) calculation.

Table S13. MS-CASPT2 Evaluated Emission Energy (eV) and Wavelength (λ /nm) in Gas Phase.

	Root 1	Root 2	E_{\perp} (eV)	λ (nm)
a	-1058.700694	-1058.596221	2.84	436
b	-1019.517768	-1019.428509	2.43	510
c	-1057.535622	-1057.465675	1.90	651
d	-944.4494865	-944.3915562	1.58	787
e	-999.6725762	-999.6155484	1.55	799
f	-969.8234327	-969.7830014	1.10	1127

Table S14. Calculated Vertical Emission Energies (E_{\perp} /eV), Wavelength (λ /nm), Oscillator Strengths (f) in Gas Phase and N,N-Dimethyl Formamide (DMF) Solution.

	E_{\perp} (eV)	λ (nm)	f
In Gas Phase			
a	2.78	446	0.0010
b	2.18	570	0.0035
c	2.07	598	0.0011
d	1.76	703	0.0183
e	1.62	766	0.0003
f	1.32	940	0.0034
g	2.70	460	0.0010
In DMF Solution			
a	2.89	429	0.0013
b	2.32	534	0.0063
c	2.18	570	0.0020
d	1.88	661	0.0300
e	1.81	684	0.0007
f	1.44	863	0.0056
g	2.89	429	0.0027
g^{σ}	3.09	401	0.0056

Note: **g**: modified BNQDs that doped C atom connects with -COOH group ^{σ} ; in aqueous solution

Table S15. Computed HOMO (H), LUMO(L) and HOMO–LUMO (H–L) Gap Energies (eV) of BNQDs **a-f** at S_0 and S_1 Minima.

Energy	S_0			S_1		
	H (eV)	L (eV)	H–L (eV)	H (eV)	L (eV)	H–L (eV)
a	–6.50	–1.34	5.16	–5.71	–1.58	4.13
b	–6.90	–1.37	5.53	–5.48	–1.87	3.60
c	–6.95	–1.31	5.64	–6.83	–3.24	3.59
d	–6.88	–0.42	6.46	–5.49	–2.48	3.00
e	–6.26	–0.96	5.30	–4.57	–1.64	2.93
f	–6.91	–1.63	5.28	–6.14	–3.56	2.58

Table S16. Computed S_r Index (a.u.), D Index (Å), H Index (Å) and t Index (Å) in Electron Excitation and Emission Process.

		S_r index (a.u.)	D index (Å)	H index (Å)	t index (Å)
a	$S_0 \rightarrow S_1$	0.51697	1.070	2.193	–0.154
	$S_1 \rightarrow S_0$	0.49168	0.841	2.250	–0.313
b	$S_0 \rightarrow S_1$	0.52475	0.704	3.709	–0.474
	$S_1 \rightarrow S_0$	0.49821	0.820	2.082	–0.303
c	$S_0 \rightarrow S_1$	0.54750	0.599	1.848	–0.478
	$S_1 \rightarrow S_0$	0.56908	0.903	1.955	–0.183
d	$S_0 \rightarrow S_1$	0.48898	1.192	3.709	–1.375
	$S_1 \rightarrow S_0$	0.53665	0.798	2.012	–0.156
e	$S_0 \rightarrow S_1$	0.50063	0.960	2.326	–0.354
	$S_1 \rightarrow S_0$	0.44864	1.380	2.060	0.184
f	$S_0 \rightarrow S_1$	0.51934	1.109	2.378	–0.194
	$S_1 \rightarrow S_0$	0.56072	1.218	2.018	–0.022

Table S17. B3LYP-D3BJ/6-311++G**/SMD Computed Total Energies (Unit: Hartree) of Doped BNQDs at the Ground State.

a	b	c
–1062.46912344	–1023.16361569	–1061.30119964
d	e	f
–947.93782325	–1003.29354447	–973.391528682