Supporting Information for

Amino Functionalization of Carbon Dots Leads to Red Emission Enhancement

Evgeny V. Kundelev,[†,*] Nikita V. Tepliakov,[†] Mikhail Yu. Leonov,[†] Vladimir G. Maslov,[†] Alexander V. Baranov,[†] Anatoly V. Fedorov,[†] Ivan D. Rukhlenko,[‡,†] Andrey L. Rogach[¶,†,*]

[†]*Information Optical Technologies Centre, ITMO University, St. Petersburg 197101, Russia*

[‡]*Institute of Photonics and Optical Science (IPOS), School of Physics, The University of Sydney, Camperdown 2006, NSW, Australia*

[¶]*Department of Materials Science and Engineering and Centre for Functional Photonics, City University of Hong Kong, Hong Kong SAR, China*

E-mail: kundelev.evg@gmail.com, andrey.rogach@cityu.edu.hk

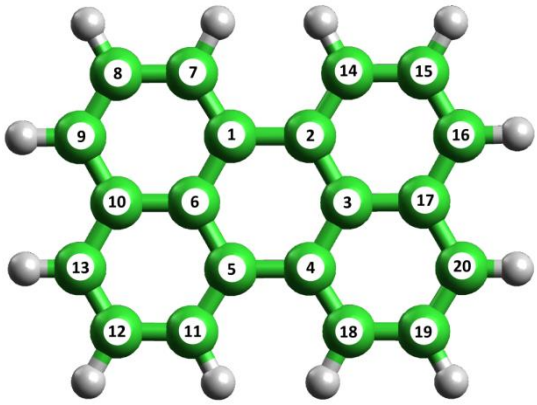

Figure S1. Geometry of perylene optimized within DFT/B3LYP/DZ approach.

Table S1. Energy, weights, and symmetry of molecular orbitals of perylene.

№	Energy (eV)	Weights	Type
4	-0.793	41(P:z-1C) 36(P:z-9C) 31(P:z-8C)	π^*
3	-0.976	32(P:z-9C) 30(P:z-1C) 23(P:z-3C) 13(P:z-7C);	π^*
2	-1.258	36(P:z-8C) 32(P:z-7C) 21(P:z-10C) 21(P:z-3C)	π^*
1	-2.752	39(P:z-9C); 36(P:z-7C); 23(P:z-1C)	π^*
0	-5.822	39(P:z-9C) 32(P:z-7C) 23(P:z-1C) 7(P:z-8C)	π
-1	-7.422	33(P:z-8C) 30(P:z-7C) 18(P:z-3C) 18(P:z-10C)	π
-2	-7.568	34(P:z-7C) 30(P:z-8C) 18(P:z-3C) 18(P:z-10C)	π
-3	-7.645	34(P:z-9C); 34(P:z-1C); 31(P:z-8C)	π

Table S2. Energies, oscillator strengths, and weights of electronic transitions for perylene in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.7937	0.566	0.99 (0→1)
2	3.7562	0	0.63(0→2) 0.34(-1→1)
3	4.0544	0.244×10^{-1}	0.65(-2→1) 0.33(0→5)
4	4.0894	0	0.50(0→3) 0.36(-1→1)
5	4.1619	0	0.57(-4→1) 0.26(0→3)
6	4.2697	0	0.65(-3→1) 0.34(0→4)
7	4.5697	0	0.39(-4→1) 0.23(-1→1)
8	4.6470	0	0.62(0→4) 0.31(-1→3)
9	4.8219	0.717	0.62(0→5) 0.31(-2→1)
10	5.5296	0.244×10^{-3}	0.51(-4→2) 0.44(-1→3)

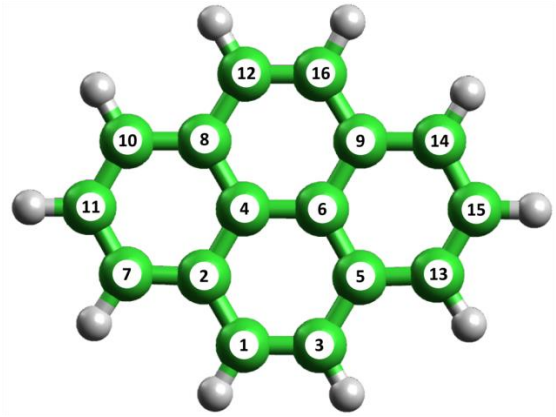

Figure S2. Geometry of pyrene optimized within DFT/B3LYP/DZ approach.

Table S3. Energy, weights, and symmetry of molecular orbitals of pyrene.

№	Energy (eV)	Weights	Type
4	-0.240	59(p_z -2C) 41(p_z -7C) 11(p_z -1C)	π^*
3	-0.865	63(p_z -1C) 42(p_z -4C)	π^*
2	-1.436	38(p_z -11C) 33(p_z -2C) 18(p_z -4C) 12(p_z -7C)	π^*
1	-2.325	57(p_z -7C) 34(p_z -1C) 15(p_z -2C)	π^*
0	-6.152	54(p_z -7C) 33(p_z -1C) 14(p_z -2C)	π
-1	-7.082	36(p_z -11C) 30(p_z -2C) 16(p_z -4C) 12(p_z -7C)	π
-2	-7.728	61(p_z -1C) 37(p_z -4C)	π
-3	-8.216	54(p_z -2C) 37(p_z -7C) 9(p_z -1C)	π

Table S4. Energies, oscillator strengths, and weights of electronic transitions for pyrene in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	3.6396	0.546	0.95 (0→1) 0.04(-1→2)
2	3.8118	0.501×10^{-3}	0.53(0→2) 0.46(-1→1)
3	4.4769	0	0.85(0→3) 0.15(-2→1)
4	4.5678	0.510	0.51(-1→1) 0.44(0→2)
5	4.6881	0	0.84(-2→1) 0.14(0→3)
6	5.1159	0	0.47(0→4) 0.46(-3→1)
7	5.3328	0	0.50(-1→3) 0.43(-2→2)
8	5.3701	1.231	0.94(-1→2)
9	5.7772	0	0.45(-3→1) 0.45(0→4)
10	6.9733	0	0.50(-2→2) 0.42(-1→3)

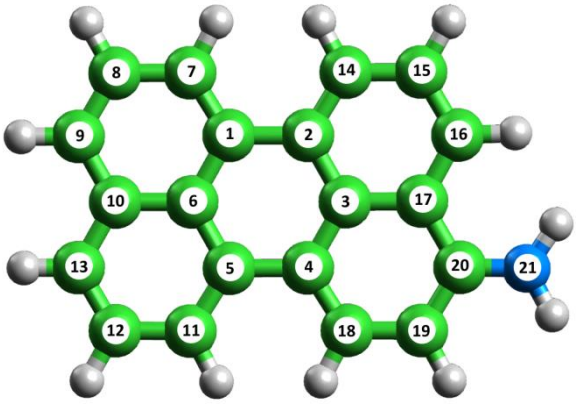

Figure S3. Geometry of Pe1 subunit optimized within DFT/B3LYP/DZ approach.

Table S5. Parameters of molecular orbitals of Pe1 subunit.

№	Energy (eV)	Weights	Type
4	-0.488	16(p_z -1C) 14(p_z -9C) 13(p_z -4C) … **3(p_z -21N)**	a_π
3	-0.744	18(p_z -5C) 16(p_z -13C) 14(p_z -2C) 12(p_z -16C)	a_π
2	-0.999	11(p_z -3C) 11(p_z -17C) 11(p_z -19C) 11(p_z -15C)	a_π
1	-2.595	13(p_z -16C) 11(p_z -9C) 11(p_z -14C) … **4(p_z -21N)**	a_π
0	-5.092	12(p_z -4C) 11(p_z -13C) **11(p_z -21N)** 10(p_z -11C)	*l*
-1	-6.710	**20(p_z -21N)** 12(p_z -1C) 12(p_z -9C) 10(p_z -19C)	*l*
-2	-7.289	16(p_z -10C) 16(p_z -6C) 15(p_z -12C) 15(p_z -11C)	*l*
-3	-7.434	16(p_z -5C) 16(p_z -13C) 15(p_z -2C) 14(p_z -16C)	*l*

Table S6. Parameters of transitions for Pe1 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.5156	0.5424	0.98(0→1)
2	3.5215	0.815×10^{-2}	0.85(0→2) 0.08(0→3)
3	3.7723	0.420×10^{-1}	0.91(-1→1)
4	3.9206	0.998×10^{-1}	0.84(0→3) 0.07(-2→1)
5	3.9810	0.204×10^{-1}	0.43(0→5) 0.19(-4→1) 0.19(-2→1)
6	4.1934	0.313×10^{-2}	0.29(0→4) 0.26(-3→1) 0.20(0→5)
7	4.3781	0.174×10^{-1}	0.45(0→4) 0.21(-2→1) 0.16(-3→1)
8	4.5501	0.846×10^{-1}	0.53(-3→1) 0.23(-2→1)
9	4.6545	0.518	0.61(-4→1) 0.25(0→5)
10	5.0653	0.129	0.88(-1→2)

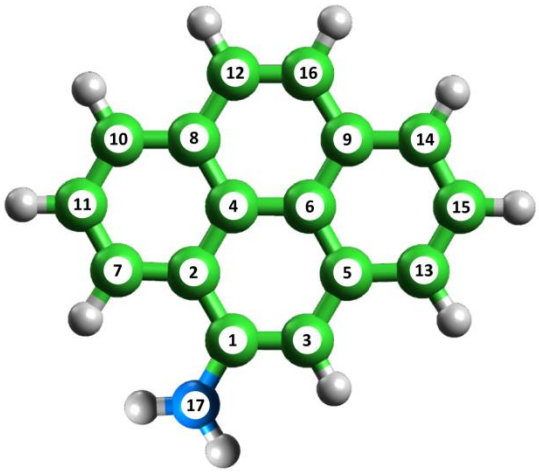

Figure S4. Geometry of Py1 subunit optimized within DFT/B3LYP/DZ approach.

Table S7. Parameters of molecular orbitals of Py1 subunit.

№	Energy (eV)	Weights	Type
4	-0.039	18(p_z -5C) 15(p_z -14C) 14(p_z -9C) … **3(p_z -17N)**	a_π
3	-0.549	22(p_z -6C) 18(p_z -4C) 18(p_z -12C) … **3(p_z -17N)**	a_π
2	-1.341	21(p_z -11C) 17(p_z -15C) 13(p_z -4C) 9(p_z -8C)	a_π
1	-2.144	16(p_z -7C) 15(p_z -10C) 12(p_z -13C) … **2(p_z -17N)**	a_π
0	-5.639	21(p_z -3C) **18(p_z -17N)** 14(p_z -14C) 12(p_z -13C)	l
-1	-6.734	15(p_z -6C) 14(p_z -12C) **14(p_z -17N)** 2(p_z -2C)	l
-2	-7.088	15(p_z -4C) 13(p_z -15C) 12(p_z -16C) … **5(p_z -17N)**	l
-3	-8.065	15(p_z -2C) 13(p_z -10C) 12(p_z -8C) … **2(p_z -17N)**	l

Table S8. Parameters of transitions for Py1 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	3.1627	0.307	0.93(0→1) 0.03(-1→1)
2	3.5884	0.431×10^{-1}	0.83(0→2) 0.09(-1→1)
3	4.1212	0.315	0.83(-1→1) 0.06(0→2)
4	4.3392	0.105	0.70(-2→1) 0.16(-1→2)
5	4.4422	0.474×10^{-1}	0.93(0→3)
6	4.8644	0.992×10^{-1}	0.51(-1→2) 0.23(0→4)
7	5.0465	0.387	0.53(0→4) 0.17(-1→2)
8	5.3714	0.602	0.58(-2→2) 0.18(-1→3)
9	5.4461	0.316	0.51(-3→1) 0.16(-2→2)
10	5.5806	0.203×10^{-1}	0.83(-4→1) 0.24(-1→3)

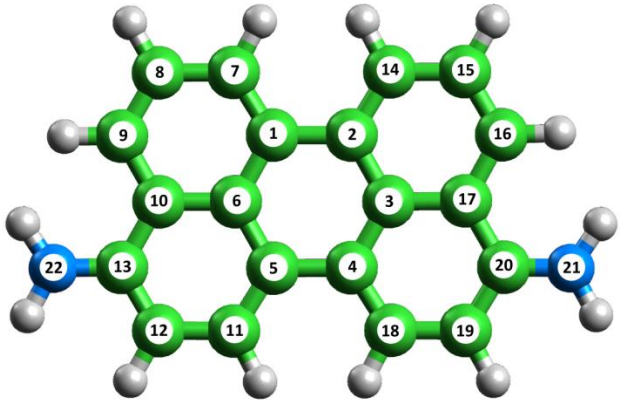

Figure S5. Geometry of Pe2 subunit optimized within DFT/B3LYP/DZ approach.

Table S9. Parameters of molecular orbitals of Pe2 subunit.

№	Energy (eV)	Weights	Type
4	-0.494	24(p_z -1C) 23(p_z -9C) 15(p_z -12C) … **3(p_z -22N)**	a_π
3	-0.565	22(p_z -8C) 21(p_z -3C) 19(p_z -11C) 17(p_z -10C)	a_π
2	-1.066	20(p_z -3C) 20(p_z -10C) 19(p_z -8C) 17(p_z -12C)	a_π
1	-2.347	26(p_z -9C) 21(p_z -7C) 16(p_z -1C) … **5(p_z -22N)**	a_π
0	-4.932	**20(p_z -22N)** 17(p_z -4C) 15(p_z -13C) 13(p_z -11C)	*l*
-1	-6.483	**34(p_z -22N)** 23(p_z -12C) 20(p_z -4C) 7(p_z -8C)	*l*
-2	-6.889	22(p_z -9C) 19(p_z -1C) **16(p_z -22N)** 14(p_z -7C)	*l*
-3	-7.253	**34(p_z -22N)** 23(p_z -12C) 20(p_z -4C) 7(p_z -8C)	*l*

Table S10. Parameters of transitions for Pe2 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.2439	0.458	0.98(0→1)
2	3.2623	0.206×10^{-2}	0.94(0→2)
3	3.5994	0.755×10^{-2}	0.92(-1→1)
4	3.7944	0.113	0.83(0→3) 0.14(-4→1)
5	3.9435	0.111×10^{-2}	0.90(0→4)
6	3.9524	0.389	0.86(0→5)
7	4.0049	0.378×10^{-1}	0.83(-2→1) 0.12(-3→1)
8	4.4006	0.456×10^{-2}	0.53(-3→1) 0.09(-2→1)
9	4.5662	0.306	0.65(-4→1) 0.19(-2→1)
10	4.8928	0.421	0.78(-1→2) 0.16(-4→1)

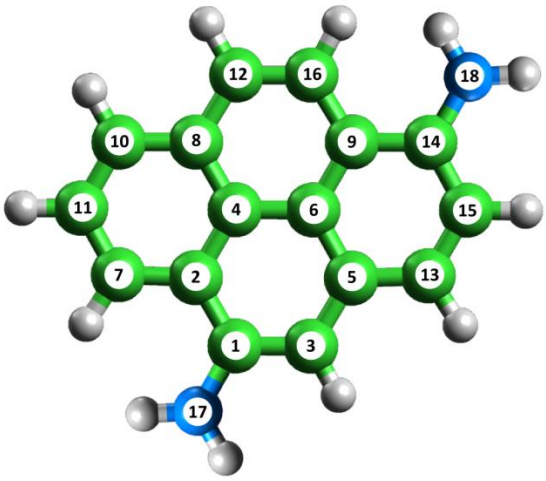

Figure S6. Geometry of Py2 subunit optimized within DFT/B3LYP/DZ approach.

Table S11. Parameters of molecular orbitals of Py2 subunit.

№	Energy (eV)	Weights	Type
4	0.303	18(p_z -2C) 13(p_z -10C) 12(p_z -3C) … **6(p_z -N)**	a_π
3	-0.448	21(p_z -4C) 18(p_z -16C) 17(p_z -6C) … **3(p_z -17N)**	a_π
2	-1.224	21(p_z -15C) 15(p_z -11C) 13(p_z -6C) 11(p_z -9C)	a_π
1	-1.913	15(p_z -14C) 15(p_z -13C) 14(p_z -7C) … **4(p_z -N)**	a_π
0	-5.057	**14(p_z -18N) 14(p_z -17N)** 12(p_z -1C) 10(p_z -10C)	l
-1	-6.600	**29(p_z -17N)** 14(p_z -16C) 13(p_z -4C) … **2(p_z -18N)**	l
-2	-6.795	24(p_z -11C) 17(p_z -1C) **11(p_z -18N)** … **4(p_z -17N)**	l
-3	-7.395	**18(p_z -18N)** 17(p_z -13C) 16(p_z -9C) 15(p_z -8C)	l

Table S12. Parameters of transitions for Py2 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.8240	0.369	0.95(0→1)
2	3.2284	0.835×10^{-1}	0.94(0→2)
3	3.9713	0.599×10^{-1}	0.95(0→3)
4	4.1259	0.146	0.93(-1→1)
5	4.3237	0.169	0.75(-2→1) 0.11(-1→2)
6	4.6557	0.565×10^{-2}	0.51(-1→2) 0.26(-3→1) 0.13(0→4)
7	4.9371	0.267	0.32(0→4) 0.27(-2→2) 0.20(-1→2)
8	4.9954	0.191	0.43(0→4) 0.25(-3→1) 0.12(-2→2)
9	5.1735	0.198×10^{-2}	0.98(0→5)
10	5.2627	0.882	0.53(-2→2) 0.23(-3→1) 0.12(-1→2)

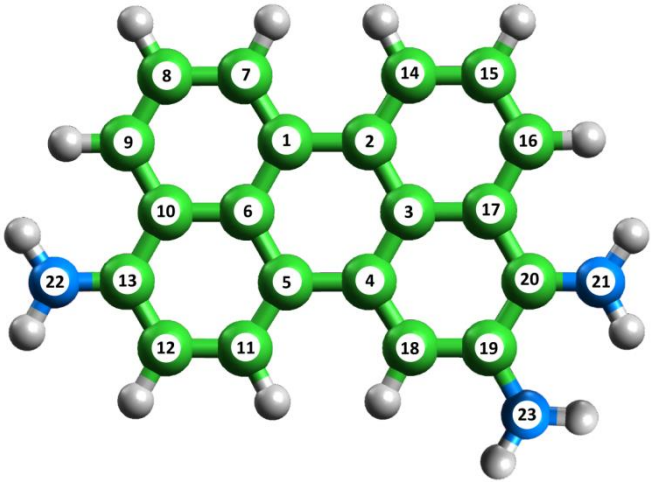

Figure S7. Geometry of Pe3 subunit optimized within DFT/B3LYP/DZ approach.

Table S13. Parameters of molecular orbitals of Pe3 subunit.

№	Energy (eV)	Weights	Type
4	-0.357	15(p_z -13C) 14(p_z -5C) 11(p_z -2C) … **5(p_z -N)**	a_π
3	-0.467	17(p_z -15C) 15(p_z -8C) 11(p_z -18C) … **1(p_z -21N)**	a_π
2	-0.935	15(p_z -10C) 14(p_z -12C) 14(p_z -6C) 14(p_z -7C)	a_π
1	-2.279	13(p_z -9C) 11(p_z -16C) 10(p_z -7C) … **5(p_z -N)**	a_π
0	-4.769	**13(p_z -21N)** 13(p_z -20C) 8(p_z -4C) … **13(p_z -N)**	l
-1	-5.861	**23(p_z -23N)** 15(p_z -18C) **9(p_z -22N)** … **6(p_z -21N)**	l
-2	-6.707	**17(p_z -22N)** 12(p_z -3C) 11(p_z -12C) … **5(p_z -N)**	l
-3	-6.870	18(p_z -17C) 18(p_z -14C) **14(p_z -21N)** … **3(p_z -N)**	l

Table S14. Parameters of transitions for Pe3 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.1388	0.387	0.98(0→1)
2	3.0927	0.706×10^{-1}	0.94(-1→1)
3	3.2706	0.548×10^{-2}	0.90(0→2)
4	3.6984	0.211×10^{-1}	0.66(0→3) 0.24(-2→1)
5	3.8611	0.237	0.84(0→4)
6	3.9097	0.217	0.69(-2→1) 0.15(0→3)
7	3.9903	0.270×10^{-1}	0.74(0→5) 0.10(-3→1)
8	4.2337	0.153	0.60(-3→1)
9	4.2921	0.598×10^{-1}	0.57(-1→2) 0.22(-4→1)
10	4.6103	0.415	0.48(-4→1) 0.32(-1→2)

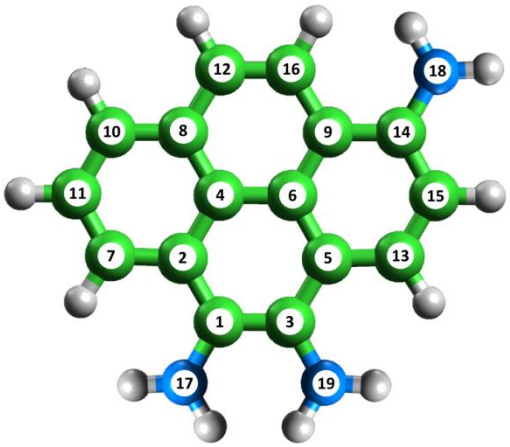

Figure S8. Geometry of Py3 subunit optimized within DFT/B3LYP/DZ approach.

Table S15. Parameters of molecular orbitals of Py3 subunit.

№	Energy (eV)	Weights	Type
4	0.348	17(p_z -5C) 12(p_z -2C) 12(p_z -13C) …**5(p_z -N)**	a_π
3	-0.345	22(p_z -6C) 19(p_z -4C) 16(p_z -12C) …**6(p_z -N)**	a_π
2	-1.147	19(p_z -11C) 17(p_z -15C) 11(p_z -8C) 10(p_z -9C)	a_π
1	-1.806	16(p_z -13C) 13(p_z -7C) 13(p_z -10C) …**5(p_z -N)**	a_π
0	-4.771	**17(p_z -17N)** 16(p_z -1C) … **12(p_z -19N) 7(p_z -18N)**	*l*
-1	-6.046	**18(p_z -19N) 17(p_z -18N)** 17(p_z -5C) … **4(p_z -17N)**	*l*
-2	-6.574	17(p_z -2C) 13(p_z -10C) 12(p_z -6C) **11(p_z -17N)**	*l*
-3	-7.270	18(p_z -7C) 18(p_z -8C) 16(p_z -9C) … **11(p_z -18N)**	*l*

Table S16. Parameters of transitions for Py3 subunit in toluene.

№	Energy (eV)	Oscillator strength	Weights
1	2.5924	0.592	0.96(0→1)
2	3.0196	0.895×10^{-1}	0.96(0→2)
3	3.6955	0.175	0.92(-1→1)
4	4.0300	0.583×10^{-1}	0.75(0→3) 0.16(-2→1)
5	4.1427	0.118	0.43(-2→1) 0.31(-1→2) 0.17(0→3)
6	4.3842	0.253×10^{-2}	0.98(0→5)
7	4.4285	0.195	0.52(-1→2) 0.28(-2→1)
8	4.6669	0.251	0.50(0→4) 0.16(-3→1) 0.15(-2→2)
9	4.7857	0.265	0.32(0→4) 0.28(-2→2) 0.27(-3→1)
10	5.1718	0.553	0.43(-2→2) 0.37(-3→1)