Supporting Information

Facile Synthesis of Halogenated of Multi-Walled Carbon Nanotubes and Their Unusual Photoluminescence

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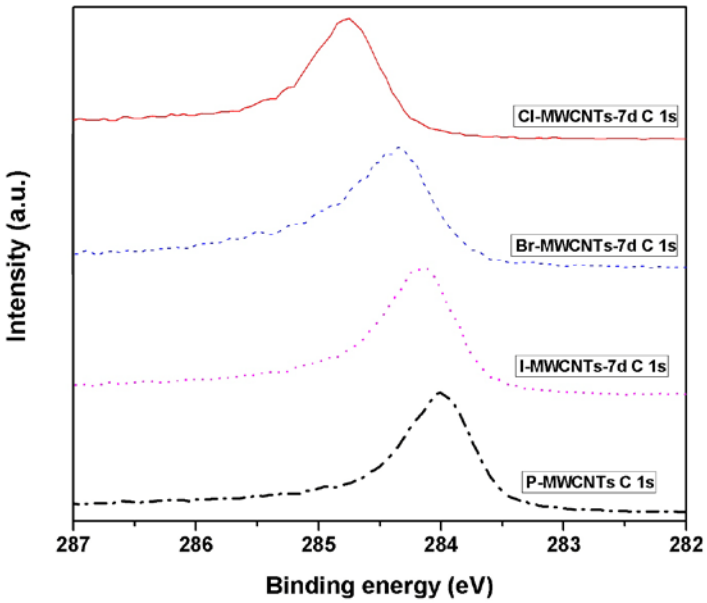

Figure S1. The C 1s XPS high-resolution spectra of pristine MWCNTs, Cl-MWCNTs, Br-MWCNTs and I-MWCNTs.

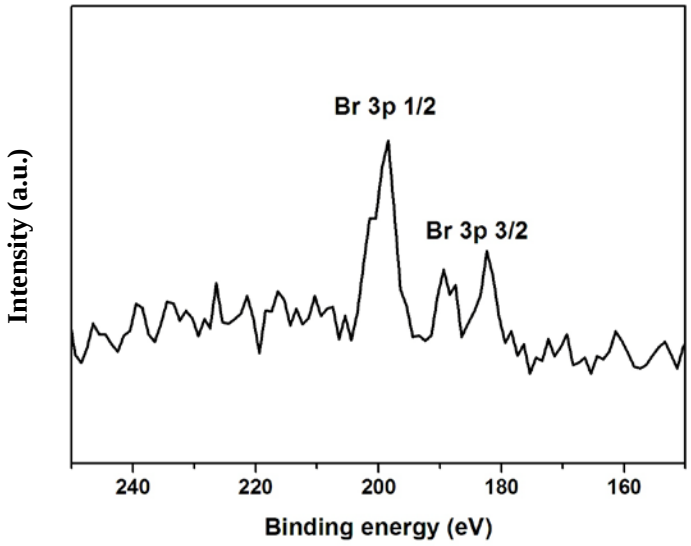

Figure S2. The selected region of Br 3p XPS spectrum of Br-MWCNTs.

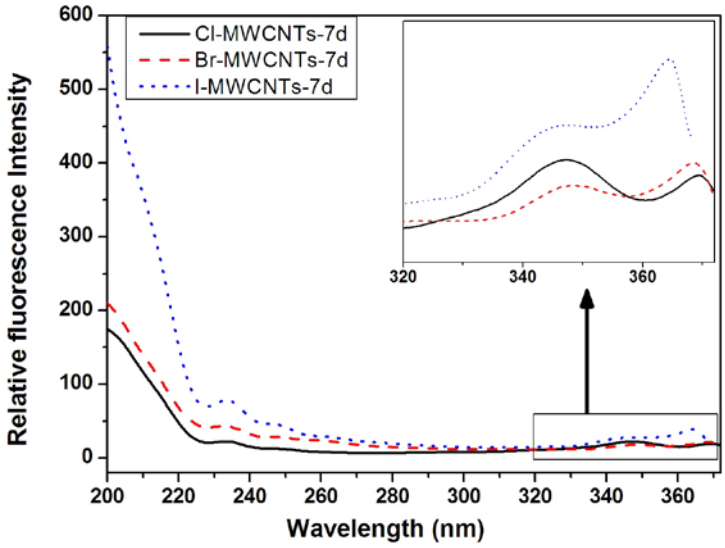

Figure S3. The excitation spectra of Cl-MWCNTs-7d, Br-MWCNTs-7d and I-MWCNTs-7d.

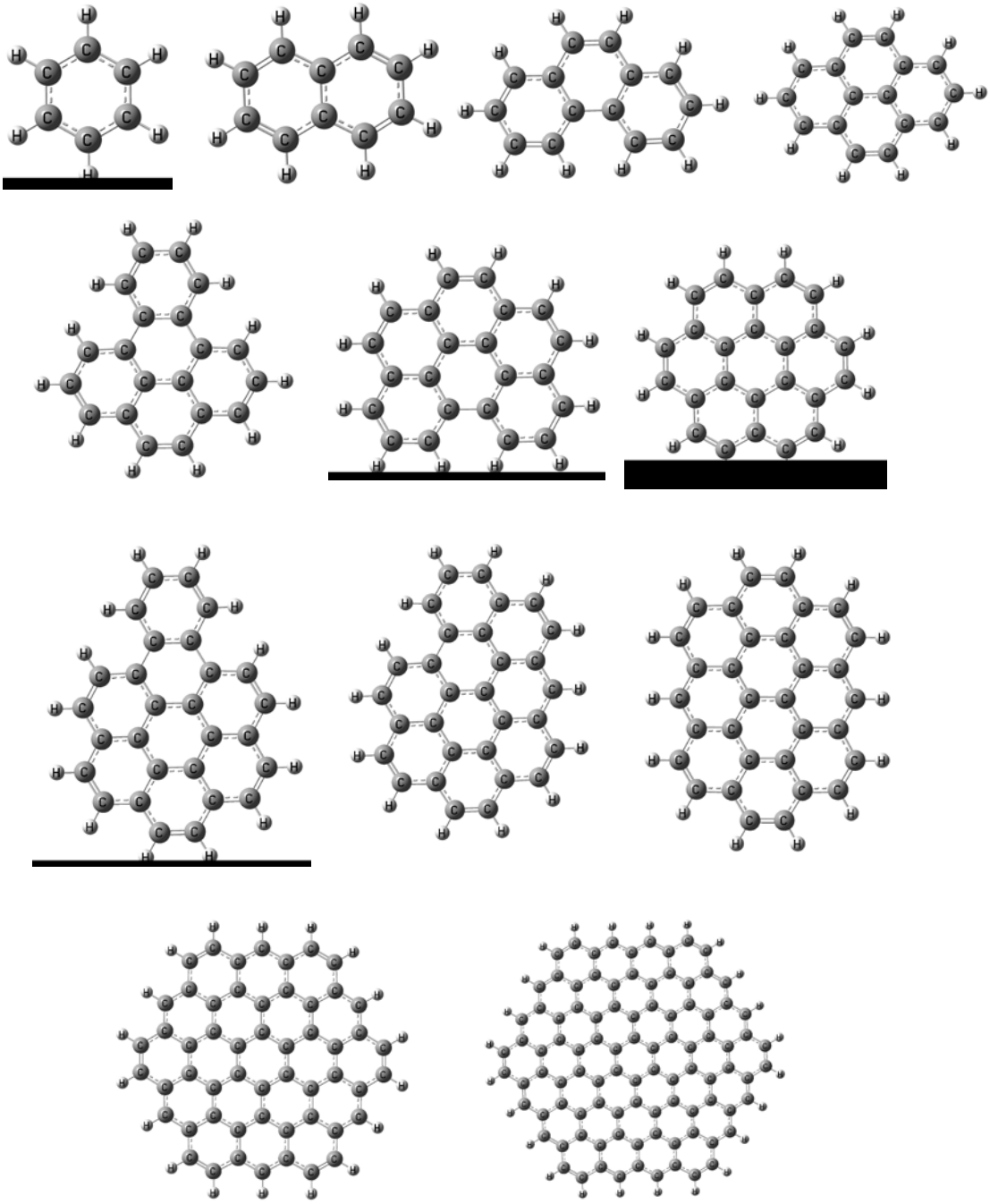

Figure S4. The structures of model compounds with different aromatic rings (N = 1 – 10, 19, 37) optimized at PBE0/6-31G(d) level

Table S1. The calculated excitation maximum wavelengths, oscillator strengths, electron transitions and emission maximum wavelengths of model compounds with 1-10, 19 and 37 aromatic rings.

N	λ_{ex}	f_{ex}	contributions to excitation maximum wavelength	λ_{em}
1	219	0.00	HOMO-1 -> LUMO -0.46170 HOMO-1 -> LUMO+1 0.19139 HOMO -> LUMO 0.19152 HOMO -> LUMO+2 0.46175	230
2	271	0.0648	HOMO-1 -> LUMO+1 0.15780 HOMO -> LUMO 0.68621	310
3	299	0.0011	HOMO-1 -> LUMO 0.45298 HOMO -> LUMO+1 0.53694	319
4	324	0.2751	HOMO-1 -> LUMO+1 -0.21555 HOMO -> LUMO 0.67262	350
5	327	0.0001	HOMO-1 -> LUMO -0.48188 HOMO -> LUMO+1 0.49889 HOMO -> LUMO+2 -0.10354	347
6	366	0.2288	HOMO-1 -> LUMO+1 -0.14938 HOMO -> LUMO 0.68665	407
7	372	0.0000	HOMO-1 -> LUMO 0.49816 HOMO -> LUMO+1 0.49825	387
8	379	0.0000	HOMO-1 -> LUMO -0.49605 HOMO -> LUMO+1 0.49805	397
9	405	0.0467	HOMO-1 -> LUMO 0.43160 HOMO-1 -> LUMO+1 -0.11342 HOMO -> LUMO 0.36259 HOMO -> LUMO+1 0.40323	436
10	440	0.1757	HOMO-1 ->LUMO+1 -0.16985 HOMO ->LUMO 0.68367	477
19	532	0.0000	HOMO-1 -> LUMO 0.49694 HOMO-> LUMO+1 0.49699	551
37	708	0.0000	HOMO-1 -> LUMO 0.49704 HOMO -> LUMO+1 0.49699	734