

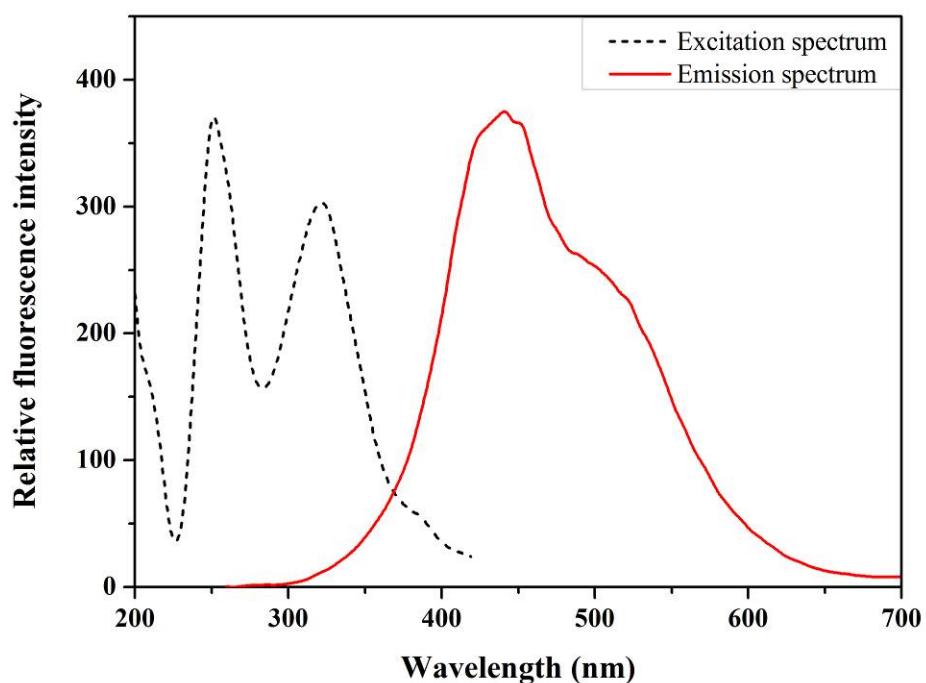
## Supporting Information

### Visible Photoluminescence Mechanism of Oxidized Multi-walled Carbon Nanotubes: An Experimental and Theoretical Investigation

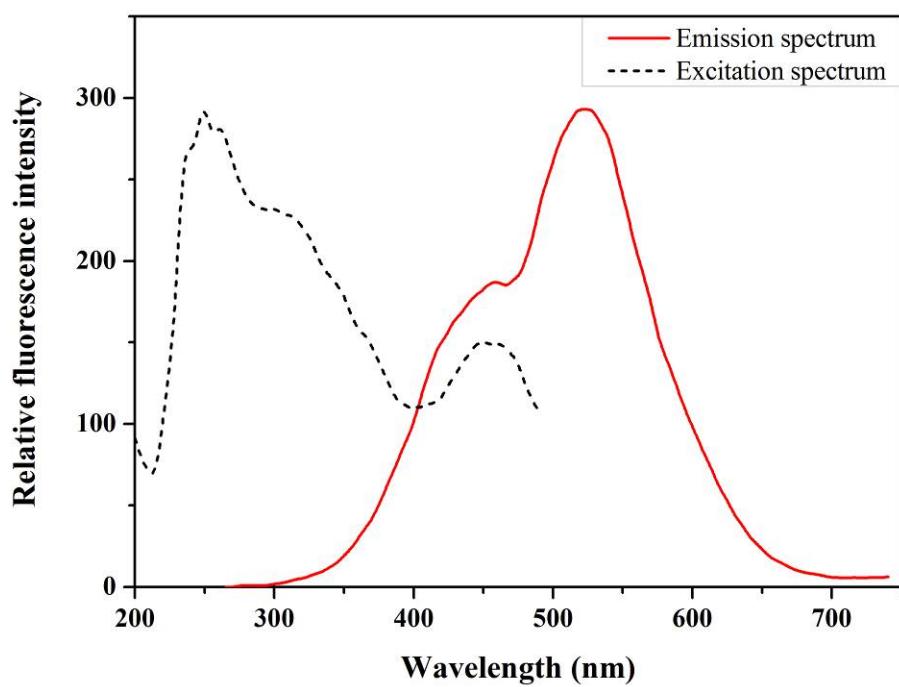
Zhaosheng Qian,<sup>‡</sup> Jin Zhou,<sup>‡</sup> Juanjuan Ma, Xiaoyue Shan, Congcong Chen, Jianrong Chen and Hui Feng\*

College of Chemistry and Life Science, Zhejiang Normal University, Jinhua 321004, P. R. China

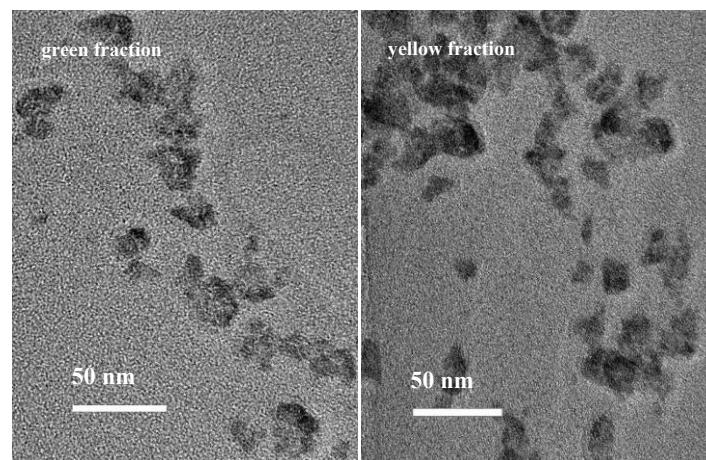
- 1. Figure S1. The excitation and emission spectra for green fraction**
- 2. Figure S2. The excitation and emission spectra for yellow fraction**
- 3. Figure. S3 HRTEM images of green fraction and yellow fraction.**
- 4. Figure S4. UV-Vis spectra of Short O-MWCNTs and Long O-MWCNTs**
- 5. Figure S5. TEM images of GO**
- 6. Figure S6. XPS spectrum of Long O-MWCNTs**
- 7. Figure S7. Structures of model compounds with 1 – 6 defects or isolated sp<sup>2</sup> carbon clusters optimized at PBE0/6-31g level**
- 8. Figure S8. HOMO and LUMO of original (6,0) SWCNT (top), compounds with six defect sites (middle) and six isolated sp<sup>2</sup> carbon clusters (bottom).**



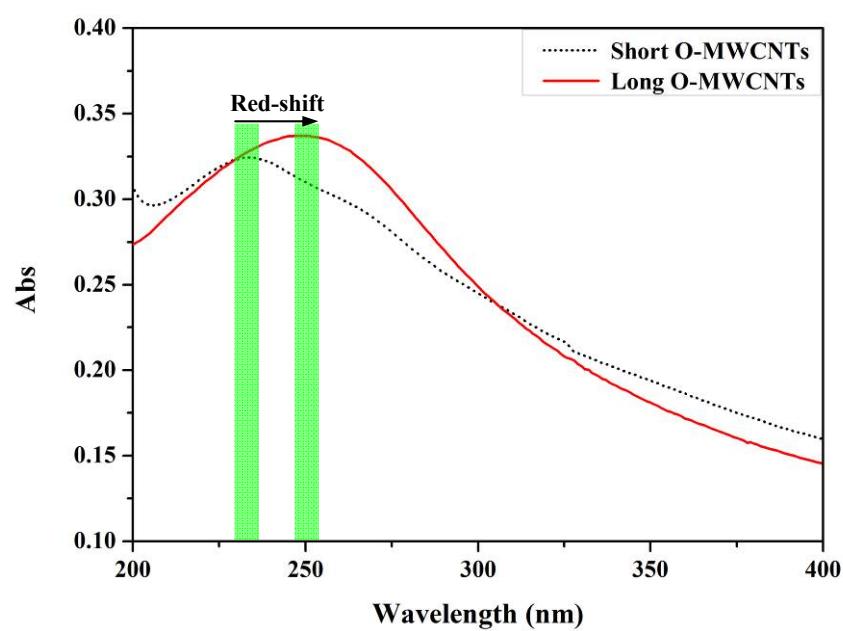
**Figure. S1** The excitation and emission spectra for green fraction



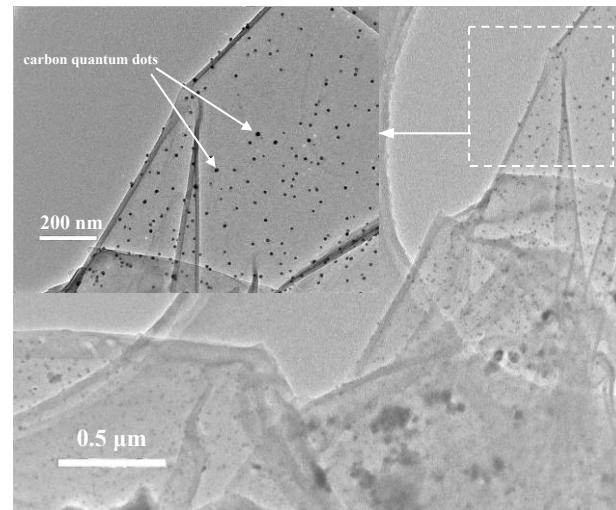
**Figure. S2** The excitation and emission spectra for yellow fraction



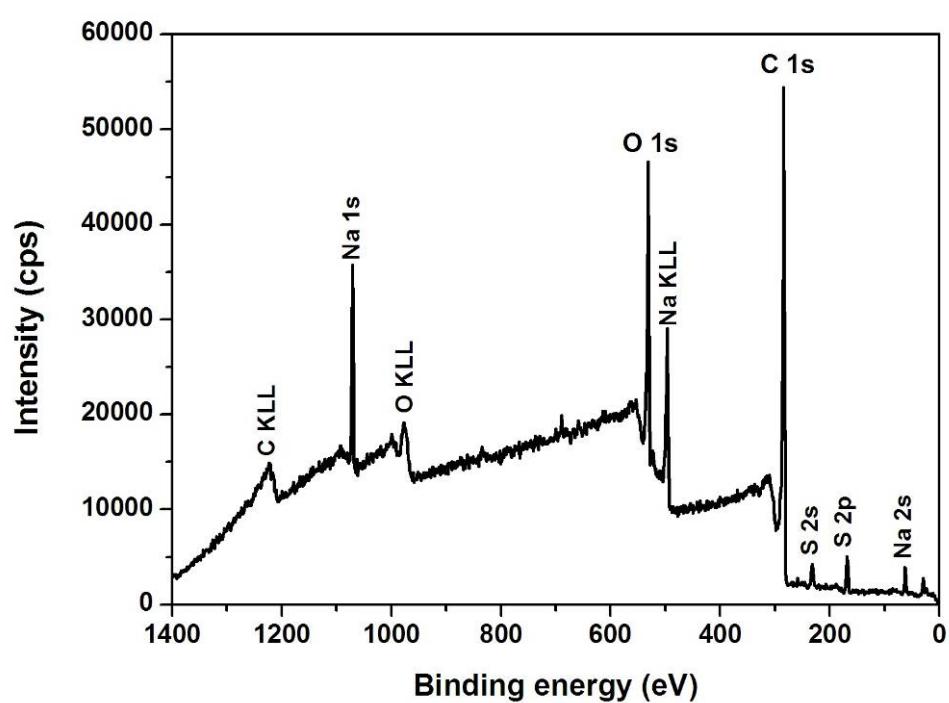
**Figure. S3** HRTEM images of green fraction and yellow fraction.



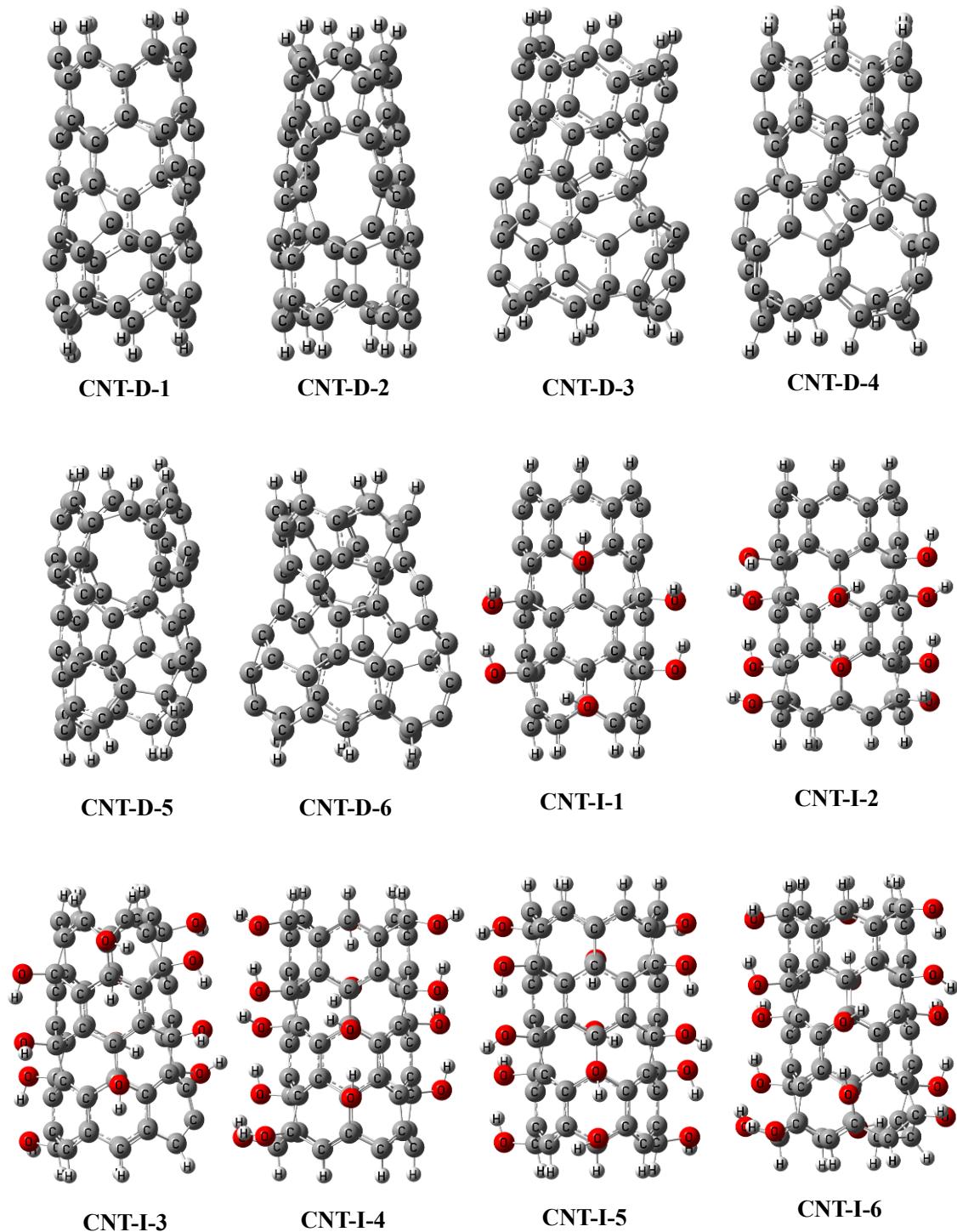
**Figure. S4** UV-Vis spectra of Short O-MWCNTs and Long O-MWCNTs



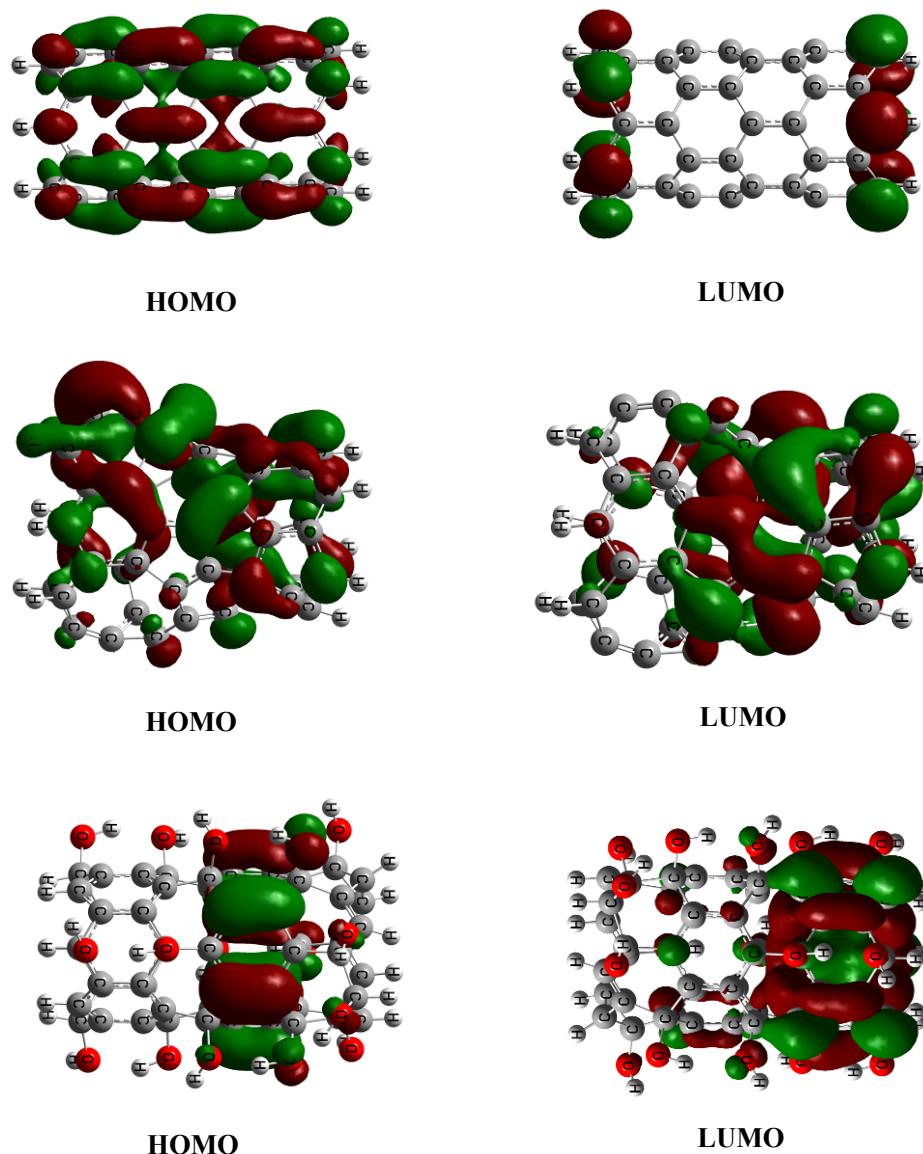
**Figure. S5** TEM images of GO



**Figure. S6** XPS spectrum of Long O-MWCNTs



**Figure S7.** Structures of model compounds with 1 – 6 defects or isolated  $sp^2$  carbon clusters optimized at PBE0/6-31g level



**Figure S8.** HOMO and LUMO of original (6,0) SWCNT (top), compounds with six defect sites (middle) and six isolated  $sp^2$  carbon clusters (bottom).