Synthesis of Benzonitrile Derivatives Appeared TADF Characteristics

Hansol Park and Min Chul Suh*
Dept. of Information Display and Advanced Display Research Center
Kyung Hee University, Seoul 130-701, Korea
Tel.:82-2-961-0694, E-mail: mcsuh@khu.ac.kr

The history of OLED has been developed from first OLED by C. W. Tang. Thermally Activated Delayed Fluorescent (TADF) OLEDs were accepted as the only way to overcome the vulnerabilities of phosphorescent OLEDs. The materials which showed TADF characteristics have something in common with low energy gap between singlet and triplet energy, spatial separation among HOMO and LUMO, and twisted angle between acceptor and donor moieties. The calculation results of these materials that we designed showed low ΔE_{ST} and reasonable LUMO & HOMO spatial separation. The procedure of these materials was quite simple and took shorter time than conventional coupling reactions. These D-A-D structured materials exhibited the range of ΔE_{ST} 0.03eV~0.04eV. The calculation results exhibited that T_1 and S_1 energies of DPtBn were 2.600 eV and 2.646 eV, and those of DPxBn were 2.285 eV and 2.316 eV respectively. The calculation results of compounds were calculated at the B3LYP/6-31G* level after optimizing molecular structure by using Gaussian 09W.

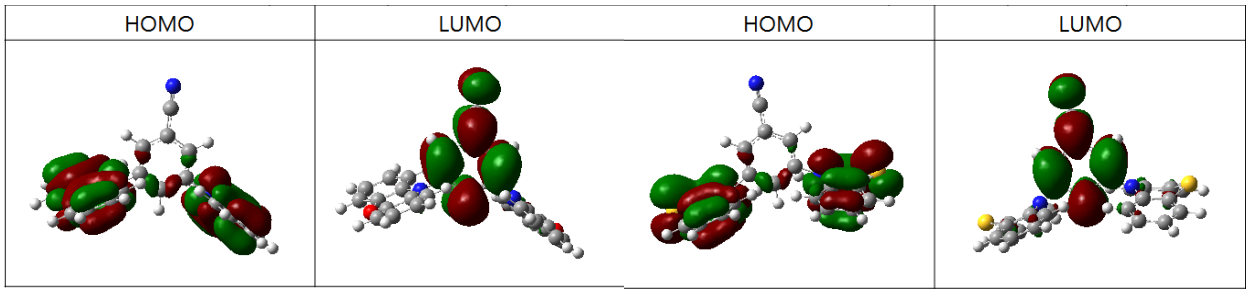

Fig.1. (Left) DPxBn's HOMO &LUMO (Right) DPtBn's HOMO & LUMO

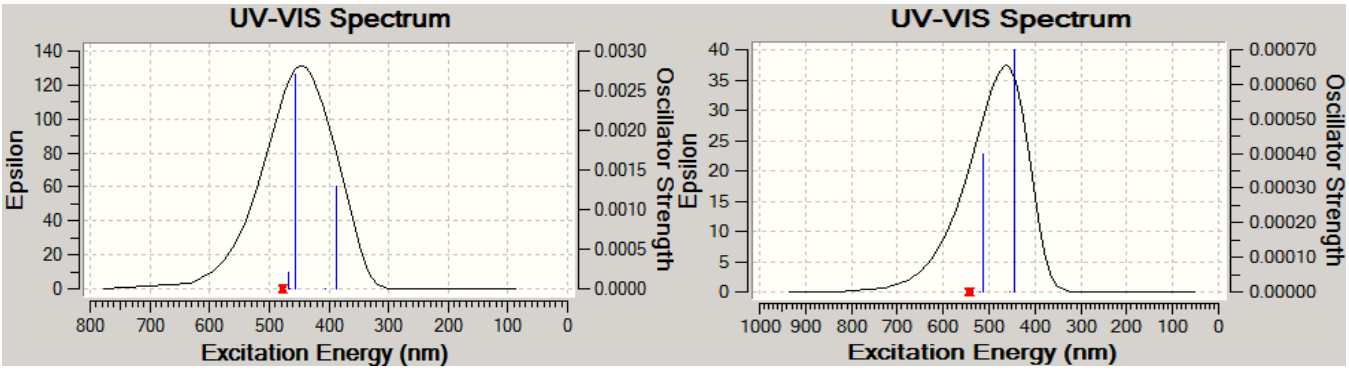

Fig.2. (Left) DPtBn's UV-Vis spectrum (right) DPxBn's UV-Vis spectrum

Acknowledgment

This work was supported by the National Research Foundation of Korea (NRF) funded by the Korea Government (MSIP) (NRF-2014R1A2A2A01002417).

References

1. Hiroki Uoyama, Chihaya Adachi, *Nature*, 492,234-238 (2012).
2. Qisheng Zhang, Chihaya Adachi, *J. Am. Chem. Soc*, 134, 14706-14709 (2012)
3. Qisheng Zhang, Chihaya Adachi, *Nature Photonics*, 8, 326-332 (2014)