Dynamics simulations of photoinduced intramolecular proton transfer reactions of 2,5-bis(2'-benzoxazolyl)hydroquinone

Rathawat Daengngern[1], Nawee Kungwan[2]

[1] Department of Chemistry, Faculty of Science,
King Mongkut's Institute of Technology Ladkrabang, Bangkok 10520, Thailand
[2] Department of Chemistry, Faculty of Science, Chiang Mai University,
Chiang Mai 50200, Thailand

E-mail: rathawat.da@kmitl.ac.th

The dynamics simulations of the excited-state intramolecular proton transfer (ESIPT) of 2,5-bis(2'-benzoxazolyl)hydroquinone (BBHQ) have been performed on their lowest energy structures using time-dependent density functional theory (TDDFT) at TD-B3LYP/SVP level.[1] Our dynamics simulations showed that the intramolecular hydrogen bond N···H−O is strengthened in the excited state, which triggers driving force to effectively facilitate the proton transfer process through an intrinsic intramolecular hydrogen bond.[2,3,4] There are two possible mechanisms of the ESIPT processes: *a*) single proton transfer and *b*) double proton transfer. The ESIPT mechanism of BBHQ systems elucidates that single proton transfer is more likely to take place in comparison with the double proton transfer reaction.[4] Moreover, the detailed information of the mechanisms and photophysical properties of these systems will be discussed.

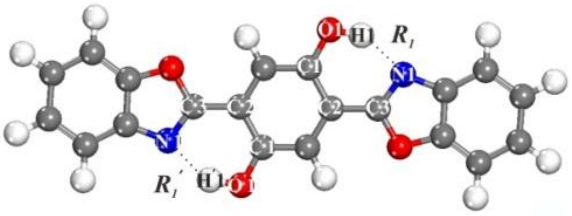

Figure 1. Optimized geometry of 2,5-bis(2'-benzoxazolyl) hydroquinone computed at B3LYP/SVP level.

Funding: King Mongkut's Institute of Technology Ladkrabang

Acknowledgement: We thank CCL-CMU at Chiang Mai University.

References:

[1] R. Daengngern, C. Prommin, T. Rungrotmongkol, V. Promarak, P. Wolschann, N. Kungwan, *Chem. Phys. Letts.*, **2016**, 657, 113
[2] N. P. Ernsting, *J. Phys. Chem.*, **1985**, 89, 4933
[3] J. Zhao, J. Chen, J. Liu, M. R. Hoffmann, *Phys. Chem. Chem. Phys.*, **2015**, 17, 11990
[4] Y. Zhang, M. Sun, Y. Li, *Sci. Rep.*, **2016**, 6, 25568