Theoretical design and study on potential organic dyes with different linkers for dye-sensitized solar cells

Ruangchai Tarsang1,*, Kanokwan Wongkam2, Siriporn Jungsuttiwong2
1Department of Science and Mathematics, Faculty of Industry and Technology, Rajamangala University of Technology Isan Sakonnakhon Campus, Sakonnakhon 47160, Thailand
2Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani 34190, Thailand
*E-mail: ruangchai.ta@rmuti.ac.th

Abstract: A series of four organic dyes containing in D-π-A-π-A architecture with different π-conjugated linkers were theoretically designed and studied by using density functional theory (DFT) and time-dependent DFT (TD-DFT). The molecular structures, absorption spectra, light-harvesting efficiency (LHE), charge density different (Δρ), charge transfer distance (dCT), adsorption energy (Eads) of dyes on the TiO2 cluster, and electron injection were systematically evaluated. The results reveal that absorption spectra are red-shifted by introducing thiophene unit as π-linkers instead of benzene unit. The organic dyes with thiophene linker exhibit not only a broader absorption spectrum, but also a higher dCT and stronger Eads values. So, in this study, the introduction of thiophene linker is the most effective strategy as a promising candidate to increase the efficiency of organic dye for dye-sensitized solar (DSSCs).

Keywords: Organic dyes; DSSCs; Solar cells; DFT calculations