Chirawat Chitpakdee 2011: Excitation Energies of Triphenylamine Cyanoacrylic Acid for Dye-Sensitized Solar Cells Using Long-Range Corrected Time-Dependent Density Functional Theory. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Songwut Suramitr, Ph.D. 60 pages.

Structures of 2-cyano-3-(4-(diphenylamino)-phenyl) acrylic acid (TC) and its derivatives were investigated using density functional theory (DFT). The structural parameters were optimized using several DFT functional, B3LYP, M06, M06-HF, M06-L, and M06-2X at 6-31G(d) basis set level. The structures obtained from various methods were used to calculate the electronic properties by TD-B3LYP/6-311G(d,p) in gas phase and compare with the experimental absorption bands. The obtained results indicate that the excitation energy from structure using M06-HF/6-31G(d) method (410 nm) is in well agreement with experimental absorption data (400 nm). Therefore, the optimized structures of TC derivatives obtained from M06-HF/6-31G(d) method are also calculated for the excitation energies using TD-DFT functional, PBE0, LC-B3LYP, LC-wPBE and CAM-B3LYP at 6-311G(d,p) level including conductor polarizable continuum model (PCM) solvation to compare with the experimental absorption bands. The results show that the absorption spectrum using the state-specific polarizable continuum model (SS-PCM) SS-PCM-TD-CAM-B3LYP/6-311G(d,p) methods (393 nm) are closer to experimental absorption data (400 nm). We conclude by discussing the benefits of theoretical calculations, which can provide critical structural and electronic understanding of electron transfer phenomena that can be exploited in design of novel optical materials.

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