Energy conversion process of substituted phthalocyanines with potential application to DSSC: a theoretical study

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A series of zinc phthalocyanine dyes with different electron-donating substituents and four types of anchor groups (described in the paper as A1, A2, A3 and A4) that interact with a semiconductor (TiO2) cluster were studied employing DFT and TD-DFT methodologies with the B3LYP hybrid functional and its long-range corrected version (CAM-B3LYP). We analyzed the range visible and near UV regions; they are the most important regions for photon to current conversion, to obtain the microscopic information about the electronic transitions and its corresponding molecular orbitals (MOs) properties. The computations provided the character of transitions involved in the studied systems. The UV?Vis spectra of the isolated dyes were obtained and compared with the computed spectra of the dyes anchored to the (TiO2)15 cluster. Furthermore, we focus on four properties that can be optimized: ?Ginj0, LHE, ?Grec0 and ?. The results obtained in this work allow us to propose the A2 as adequate anchor when ?N(CH3)2 is the substituent R. That is of potential interest for designing highly efficient dye-sensitized solar cells. © 2018, Springer-Verlag GmbH Germany, part of Springer Nature.

DFT

DSSC

Phthalocyanine

Sensitizers

TD-DFT