Molecular Design of the Carbazole-Carbazole Based Dyes for Dye-Sensitized Solar Cells: Linker Type Effect

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A series of metal-free organic donor–π–acceptor dyes [1] are assembled as organic sensitizers for application in dye-sensitized solar cells (DSSCs) and investigated by means of a combination of density functional theory (DFT) and time-dependent DFT (TDDFT) approaches. In these Carbzole-based dyes, we use Carbazole-Carbazole (CC) and cyanoacrylic acid (A) moieties as double donor and acceptor units, respectively [2]. The varied π-linker units in the designed CCXA dyes are Thiophene(CCTA), Furan(CCOA), Pyrrole(CCNA), Phenyl(CCPA), 2,1,3-Benzothiadiazole (CCBA) and Thieno[3,2-b]thiophene(CCTTA). The effects of those different π-linker units on optimized geometries, charge distributions, electronic structures, spectra and electrochemical properties of the designed organic dyes are demonstrated. All of studied systems have similar inter-ring bond lengths and dihedral angles indicate to non-planar conjunction between Carbazole and π-linker unit except for CCOA dye that has coplanar linked moieties. In all studied complexes, the HOMO molecular orbital contributions are located on the Carbazole-Carbazole donor and the LUMO contributions are primarily localized on cyanoacrylic acid acceptor. Moreover charge density difference plots also confirm the intramolecular charge transfer as desired in these donor–π–acceptor dyes. From the theoretical examination of some additional key parameters including red-shifted maximum adsorption wavelength, oscillator strength and light-harvesting efficiency, CCTTA containing a thieno[3,2-b]thiophene moiety has a balance of those fundamental factors. Among studied dyes, CCTTA is expected to be a promising initiative choice with desirable energetic and spectroscopic parameters in the DSSC field.

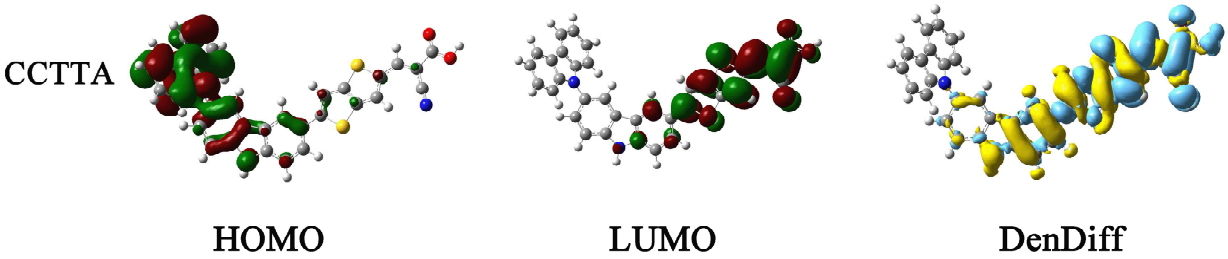

Figure 1: HOMO (left) LUMO (middle), and charge density difference (bottom) between the excited and ground states of the CCTTA dye.

References

1. M. Grätzel, J. Photochem and Photobio C: Photochem Rev. **4**, 145 (2003).
2. Feng, J., Jiao, Y., Ma, W., Nazeeruddin, M. K., Grätzel, M., Meng, S, J. Phys. Chem. C. **117**, 3772 (2013).