Predicting and improving the photovoltaic performances of phosphonic acid-based dyes sensitizers on (TiO2)9 by including an electron-withdrawing moiety

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Abstract

In this study, three novel sensitizers with the donor-acceptor-π-spacer-acceptor D-A'-π-A) structure were designed based on the benzothiadiazole (BTD) surrounded by two thiophenes in each side (T4) mono-functionalized by an acid phosphonic (A) T4BTD-A dye by insertion of vinyl and cyanide CN electron-withdrawing moiety in a different position. Their geometrical, electronic and photovoltaic parameters were predicted using density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations, via the functional BHandH in combination with the Poples basis set 6-311G(d) for small atoms and pseudo-potential basis set LANL2DZ for Titanium atom at the chloroform solvent medium via the implicit CPCM model. Results showed that the inclusion of the C=C and the CN moieties exhibits a decrease in the HOMO–LUMO gap, and a redshift in the absorption spectra. The photoelectric conversion efficiency (PCE) for the T4BTD-A dye was estimated to be about 6.57 % under the standard AM 1.5G solar radiation, which is in excellent agreement with its measured value of 6.40 %, suggesting that our calculations scheme is consistent. Moreover, the predicted PCE value after elongation of T4BTD-A by C=C and CN has increased to 7.11 % and (7.82 %, 8.09 %) respectively. Our results revealed that the addition of CN electron-withdrawing moiety enhances the PCE of the studied dyes, while the position of CN moiety has a slight effect on the PCE of the studied dyes. Additionally, our calculation suggests that the CCCN1 and CCCN2 are good candidates as efficient sensitizers for dye-sensitized solar cell DSSCs applications.

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