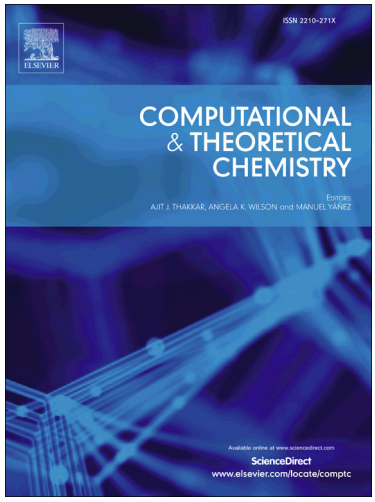


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# Theoretical investigation effects of anchor groups on photovoltaic properties for the C217-based dye sensitizer

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**ABSTRACT** Designing and synthesizing high-performable dye sensitizers has kept an important and hot issue in dye-sensitized solar cells (DSSCs). In this work, with the $(TiO_2)_{16}$ cluster, we theoretically investigated the effects of five different anchor groups (-CONHOH, -CSSH, -OH, $-PO_3H_2$, and $-SO_2H$) on the photovoltaic properties of the C217 dye by means of density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations coupled with the incoherent charge-hopping model. Results showed that the -CSSH can remarkably narrow the HOMO-LUMO gap, and enhance the dye absorption for the solar radiation. Inversely, the -OH enlarges the HOMO-LUMO gap, and induces the weaker harvest for the sun light. Using the bidentate adsorption model, the power conversion efficiency (PCE) for the C217-$(TiO_2)_{16}$ system was predicted to be as high as 9.72%, which was in excellent agreement with its measured value (9.80%). More interestingly, the DSSC based on the 2-$(TiO_2)_{16}$ system was found to possess an high open-circuit voltage of 0.782V, large short-circuit photocurrent density of 25.08mA·cm$^{-2}$ and high fill factor of 0.767, corresponding to a higher PCE of 15.04% than the C217-$(TiO_2)_{16}$, denoting the 2-$TiO_2$ system is a very promising DSSC candidate, and is worth further experimental study.

**Keywords:** anchor groups, density functional theory, C217, photovoltaic properties, dye sensitizer

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