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

Caibin Zhao* Xiaohua Guo Jianqi Ma Hongguang Ge* Lingxia Jin Qiang Zhang*

Shaanxi Key Laboratory of Catalysis, School of Chemical and Environmental Science, Shaanxi Sci-Tech University, Hanzhong, Shaanxi 723001, PR China

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 $(\text{TiO}_2)_{16}$ cluster, we theoretically investigated the effects of five different anchor groups (-CONHOH, -CSSH, -OH, $-\text{PO}_3\text{H}_2$, and $-\text{SO}_2\text{H}$) 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- $(\text{TiO}_2)_{16}$ 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- $(\text{TiO}_2)_{16}$ system was found to possess an high open-circuit voltage of 0.782V, large short-circuit photocurrent density of $25.08\text{mA}\cdot\text{cm}^{-2}$ and high fill factor of 0.767, corresponding to a higher PCE of 15.04% than the C217- $(\text{TiO}_2)_{16}$, 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

* Corresponding Author.

E-mail address: zhaocb@snut.edu.cn (C. Zhao), gehg@snut.edu.cn (H. Ge), zhangqiang22@snut.edu.cn (Q. Zhang).

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