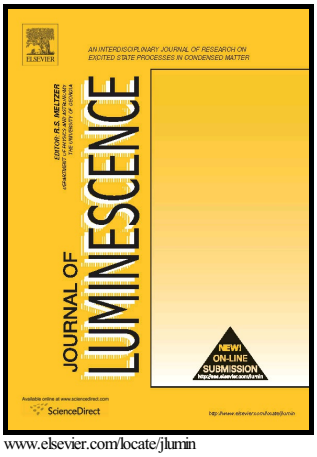
The effects of dye aggregation on the performance of organic dyes in dye-sensitized solar cells: From static model to molecular dynamics simulation

Weiyi Zhang, Yue Zhang, Huishuang Su, Xinrui Zhu, Li Wang, Jinglai Zhang



www.elsevier.com/locate/jlumin

PII: S0022-2313(18)30859-7
DOI: https://doi.org/10.1016/j.jlumin.2018.08.084
Reference: LUMIN15882

To appear in: *Journal of Luminescence*

Received date: 15 May 2018
Revised date: 3 August 2018
Accepted date: 30 August 2018

Cite this article as: Weiyi Zhang, Yue Zhang, Huishuang Su, Xinrui Zhu, Li Wang and Jinglai Zhang, The effects of dye aggregation on the performance of organic dyes in dye-sensitized solar cells: From static model to molecular dynamics simulation, *Journal of Luminescence,* https://doi.org/10.1016/j.jlumin.2018.08.084

The effects of dye aggregation on the performance of organic dyes in dye-sensitized solar cells: From static model to molecular dynamics simulation

Weiyi Zhang, Yue Zhang, Huishuang Su, Xinrui Zhu, Li Wang*, Jinglai Zhang*

College of Chemistry and Chemical Engineering, Henan University, Kaifeng, Henan 475004, P.R. China

chemwangl@henu.edu.cn
zhangjinglai@henu.edu.cn

*Corresponding authors

Abstract

The properties of three D1-π-D2-A dyes with dithiafulvenyl as donor (D1), phenothiazine as ancillary donor (D2), cyanoacrylic acid as acceptor along with different π groups, diphenyl for **1**, dithienyl for **2**, and thiopheneyl-benzothiadiazole for **3**, are studied. Besides the isolated dyes, the monomeric and dimeric adsorptions are also studied by combination of first principle and molecular dynamic simulations. There is no distinct difference among three dyes on the basis of only isolated dyes. When the dye-TiO_2 adsorption is considered, **3** is excluded because of its inferior items. However, it is still a difficult task to differentiate **1** and **2** even if the aggregation effect is included. The fluctuation of **1** is larger than that of **2** during the dynamic simulation resulting in the larger electronic coupling. The aggregation, especially for the aggregation during the dynamic simulation, is necessary to evaluate the performance of organic dye. Additionally, a new D-π-A dye **4** with the identical donor, π-bridge and acceptor is designed to compare with **2**. **2** is totally superior to **4**