Accepted Manuscript

Research paper

Controlling the charge transfer and recombination dynamics in hollow ZnO QD based dye sensitized solar cell: an insight from *ab initio* simulation

Md Habib, Narendra Nath Ghosh, Ritabrata Sarkar, Anup Pramanik, Pranab Sarkar, Sougata Pal

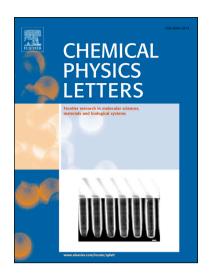
PII: S0009-2614(18)30663-8

DOI: https://doi.org/10.1016/j.cplett.2018.08.036

Reference: CPLETT 35866

To appear in: Chemical Physics Letters

Received Date: 18 June 2018 Revised Date: 11 August 2018 Accepted Date: 14 August 2018



Please cite this article as: M. Habib, N. Nath Ghosh, R. Sarkar, A. Pramanik, P. Sarkar, S. Pal, Controlling the charge transfer and recombination dynamics in hollow ZnO QD based dye sensitized solar cell: an insight from *ab initio* simulation, *Chemical Physics Letters* (2018), doi: https://doi.org/10.1016/j.cplett.2018.08.036

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Controlling the charge transfer and recombination dynamics in hollow ZnO QD based dye sensitized solar cell: an insight from *ab initio* simulation

Md Habib^a, Narendra Nath Ghosh^a, Ritabrata Sarkar^a, Anup Pramanik^b, Pranab Sarkar^b, Sougata Pal*^a

^aDepartment of Chemistry, University of Gour Banga, Malda - 732103, India ^bDepartment of Chemistry, Visva-Bharati University, Santiniketan - 731235, India

Abstract: First principle calculations are performed to study the charge transfer and recombination dynamics at the interface of dye-(ZnO)_n hollow quantum dot (QD). It has been revealed that the extent of dye-ZnO interaction depends on the size of the QD which severely affects the driving force for charge transfer and recombination. The deep level conduction band of a particular sized-QD, (ZnO)₃₆ effectively couples with the donor orbital of dye resulting faster charge injection and slower recombination which demonstrates that the size of the QD is pivotal for determining the performance of such devices.

Keywords: DSSC; ZnO hollow QD; ultrafast charge transfer; charge recombination

Corresponding Author

*E-mail: sougatapal_1979@yahoo.co.in; sougata@ugb.ac.in

Download English Version:

https://daneshyari.com/en/article/8943064

Download Persian Version:

https://daneshyari.com/article/8943064

<u>Daneshyari.com</u>