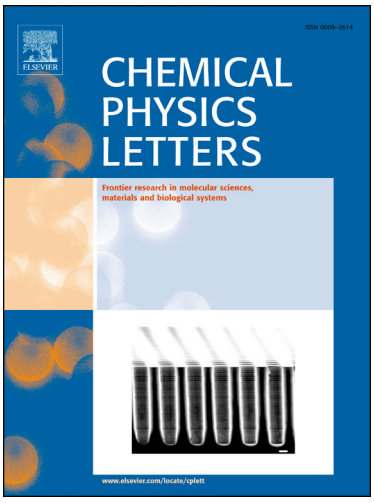

Research paper

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

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

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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

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