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Ab initio Simulations of charge transfer properties at Quantum Dot/TiO₂ Interface in Quantum Dot-Sensitized Solar Cells XUKAI XIN, Georgia Institute of Technology, RANA BISWAS, Iowa State University, ZHIQUN LIN, Georgia Institute of Technology — Quantum dot-sensitized solar cells (QDSSCs) have emerged as a very promising solar architecture for next generation photovoltaics. The QDSSCs exhibit a remarkably fast electron transfer from the quantum dot (QD) donor to the TiO₂ acceptor with size quantization properties that allows for the modulation of QD band gaps to control the photoresponse and photoconversion efficiency of QDSSCs. To understand the mechanisms that underpin this rapid charge transfer, the electronic properties of CdSe and PbSe QDs on the TiO₂ substrate were simulated using a rigorous ab initio method. In contrast to the plane wave approaches, this method capitalized on localized orbital basis set that is computationally less intensive, and provides excellent electronic structure of the constituent systems. We consider QDs grown on TiO₂ without functional ligands passivating the QD surface. We find a remarkable set of electron bridging states between QDs and TiO₂ occurring via the strong bonding between the conduction bands of QDs and TiO₂. Such bridging states account for the fast adiabatic charge transfer from the QD donor to the TiO₂ acceptor, and may be a general feature for other strongly coupled donor/acceptor systems and nanostructured semiconductor interfaces.

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