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Charge transfer between a CdSe/CdS quantum rod and an attached ferrocene molecule: a first principle study KARTICK TARAFDER, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA-94720 — Semiconductor quantum dot (QD) shows interesting opto-electrical properties, very different from bulk semiconductors. However, one major challenge for opto-electrical application is to get the charge carrier out of the QD. One approach is to use an attached molecule to extract the photon generated carrier from the QD. Ferrocene has a potential to change its electron transition level either by adjusting the Ferrocene and Ferrocene+ ratio in a solvent, or by adding other functional groups. However, proper understanding of the interactions between QD and molecule is limited, which is extremely useful for further design of such system. One of the main difficult is that there are thousands of atoms contained in the system, a first principle study of which is beyond the limit of existing computational power using direct density functional theory method. In this work we used a novel technique called charge-patching method [1], and combined that with Marcus model to study the electron and hole transfer between ferrocene and CdS/CdSe core-shell quantum dot. This study allows us to gain insights into the molecule dot interactions and underlying photoluminescence quenching process.

[1] L-W Wang, Phys. Rev. B 65, 153410(2002)

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