Abstract Submitted
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**Charge transfer between a CdSe/CdS quantum rod and a tethered ferrocene molecule**[1] LINWANG WANG, KARTICK TARAFDER, YOGESH SURENDRANATH, JACOB OLSHANSKY, PAUL ALIVISATOS, Lawrence Berkeley National Laboratory — Hole transfer between a CdSe/CdS core/shell semiconductor nanorod and a surface-ligated alkyl ferrocene is investigated by a combination of ab initio quantum chemistry calculations and experimental measurements. The calculated driving force for hole transfer corresponds well with electrochemical measurements of nanorods partially ligated by 6-ferrocenylhexanethiolate. The calculations and the experiment suggest that the hole transfer from the valence band maximum to ferrocene is through a direct coherent hopping, not through any intermediate steps, and this hopping is in the Marcus inverted region. The calculated rate of hole transfer is in line with the photoinduced hole transfer rate determined experimentally, and the calculated state energy alignment agrees excellently with the experiments. Together, the calculations suggest that holes may be extracted more efficiently from well-passivated nanocrystals by reducing the energetic driving force for hole transfer, thus minimizing energetic losses.

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