Title: A Computational Study of Optoelectronic Properties of Quantum Dots Functionalized by Ru(II) Complexes

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Metal complexes such as Ru(II)-bipyridine are well known for their oxidation and charge-transfer ability with promising applications in energy conversion. Using density functional theory (DFT) and time dependent DFT (TD-DFT), we studied the electronic structure and absorption spectra of the PbSe and ZnO quantum dot (QDs) functionalized by Ru(II)-bipyridine derivatives. The strongest QD-complex interaction is provided via the bridging attachment of the Ru(II)-complex to the QD via carboxylic linker, where each oxygen was bound to one metal atom (Pb or Zn) on the QD surface. The Ru(II)-complex introduced unoccupied molecular orbitals at the very edge of the band gap of the QD, while occupied orbitals are deep inside in the valance band, independent on the host material of the QD. The energetic alignment of complex and QD states support a scenario of electron transfer from the photoexcited complex to the QD, while the hole transfer from the photoexcited QD to the complex is highly unlikely.