

CdSe quantum dot/carbon nanotube hybrid photovoltaic systems

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CdSe quantum dot/carbon nanotube (QD/CNT) heterojunctions are one approach to creating hybrid organic/inorganic photovoltaics which combines the tunable band gap of the QDs with the high carrier mobility of CNTs. The QDs are grown in solution and capped with the ligand oleic acid. Recent edge X-ray absorption fine structure data indicate that ultrasonication of oleic acid capped QDs with acid treated multi-wall CNTs leads to strong binding of the QDs to CNTs [1]. Our first principle calculations describe the binding geometries and mechanisms involved. A strong defect enhanced binding of the QDs to CNTs via -COOH ligands is found. The enhancement is an indirect effect where structural rearrangements in the defect region of the CNTs enhances the binding energy. In terms of electronic structure, due to a negligible band gap in MWNTs with a large diameter, both the highest occupied state and lowest unoccupied state of the QDs sit in CNT bands and overlap energetically with CNT states. The question is then if one can actually use this system for a photovoltaic device: only if the tunneling rates of electrons and holes from the QD to the CNT are significantly different can one effect charge separation, and we discuss our present findings from first principles simulations.

[1] S. Azoz et al. (to be published).