

## New Design Approach for Quantum Dot Solar Cell

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Increased energy demand requires new technologies for manufacturing cheap solar cell devices. Different approaches have been attempted in order to fabricate effective and low-cost solar cell structures. One of this approaches is to use quantum dots (QDs) as light absorber, titanium dioxide ( $\text{TiO}_2$ ) as n-type semiconductor and p-type semiconducting polymers as electrode for hole conduction. The interface between the n-type semiconductor and the quantum dot (light absorber) is ensured by polyfunctional ligands (linkers), able to interact with both the  $\text{TiO}_2$  layer and the quantum dots.

In this paper, we propose the selection of quantum dots, linkers, and p-type semiconducting polymers according to the Hard Soft Acids Bases Lewis rule (HSAB) [1], according to which hard bases prefer to bond to hard acids, while soft bases prefer soft acids. The selected quantum dots are CdS, CdSe, CdTe. The proposed ligands are three aminoacids: cysteine, homocysteine and isocysteine. These ligands have mercapto groups, which ensure the interface with the QDs, and carboxylic acid groups, that ensure the interface with  $\text{TiO}_2$ . According to the HSAB rule,  $\text{Cd}^{2+}$  cations present at the surface of the QDs are soft acids and prefer to bond with the mercapto groups, which are soft Lewis bases. The interaction between  $\text{TiO}_2$  and the polyfunctional linker can be either ionic or covalent. This could be beneficial for the solar cell structure design and performance. The nature of the  $\text{TiO}_2$  - polyfunctional ligand interaction can be controlled by varying the pH of the solution. Cysteine, homocysteine and isocysteine are amphoteric molecules (having both basic and acidic properties). In acidic medium ( $\text{pH} < 1$ ), these aminoacids are mostly in cationic form (the deprotonation of the carboxylic group is prevented). Thus, a covalent bond can be generated by the esterification of the carboxylic group and of the hydroxyl group of  $\text{TiO}_2$ . In basic medium ( $\text{pH} > 12$ ), these aminoacids are presented mostly in anionic form. The carboxylic groups are deprotonated, generating carboxylate groups ( $\text{COO}^-$ ), which have ionic interaction with  $\text{Ti}^{4+}$ .  $\text{Ti}^{4+}$  is a surface defect in  $\text{TiO}_2$  that introduces specific energy levels in the  $\text{TiO}_2$  electronic density of states. According to the HSAB theory,  $\text{COO}^-$  are hard bases and  $\text{Ti}^{4+}$  are hard acids, thus having a strong interaction.

For the p-type semiconducting polymers, we suggest the use of poly 3-6mercaptohexyl thiophene, poly 3-11mercaptoundecyl thiophene and poly 3-12 mercaptododecyl thiophene, all of them containing mercapto groups as anchors that ensure the link with the QDs.

### References

1. R. G. Pearson, *Hard and soft acids and bases*, J. Am. Chem. Soc., 85 (22), 3533.