Annals of the Academy of Romanian Scientists
Series on Science and Technology of Information
ISSN 2066 - 2742 Volume **6**, Number **1/2013**

QUANTUM DOT SOLAR CELL. AN HSAB PERSPECTIVE

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Abstract *The Hard Soft Acid Base (HSAB) theory is presented as a new tool for the design of quantum dot based solar cells comprising TiO_2 / bifunctional linker / quantum dot / p-type semiconducting polymer. Since Ti^{4+} is classified as a hard acid and most of the transition metal semiconductor cations on the surface of the quantum dots are soft acids, the main goal of the discussed approach is to select bifunctional linkers with appropiate anchors for assembling quantum dots onto the surface of titania. A plethora of bifunctional ligands which belong to several classes of organic compounds (amino acids, antibiotics, vitamins, seleno compounds, etc.) are discussed and analysed in terms of the HSAB concept. The functionalization of a p-type semiconducting organic polymer backbone with an HSAB-appropiate anchor for improving the design of polymer - quantum dots hybrid interface in the solar cell structure is also presented.*

Keywords: HSAB (Hard Soft Acid Base) concept, bifunctional ligand, anchor, quantum dots, solar cells

1. Introduction

Hard Soft Acid Base (HSAB) principle was introduced by Ralph Pearson [1] in the early nineteen sixties to explain chemical reactivity of different species, the stability of different complexes, preferences of some compounds to react with other compounds, reactions mechanisms, etc. The principle applies to Lewis acids and bases, a well – known classification, according to which a molecule capable to accept an electron pair is an acid, while a molecule capable to donate it is a base.

Soft acids and soft bases exhibit the following features: strong polarizability, low electronegativity, low or zero oxidation state and large atomic/ionic radius. Examples of soft acids are: CH_3Hg^+, Pt^{2+}, Pd^{2+}, Ag^+, I_2, trinitrobenzene, carbenes, metal atoms, tetracyanoethylene, Au^+, Hg^{2+}, GaI_3, Hg_2^{2+}, Cd^{2+}, BH_3. Examples of soft bases include: benzene, ethylene, R_3P, SCN^-, I^-, RSH, R_2S, R_3As, CO.

By contrast, hard acids and bases tend to have a smaller ionic/atomic radius, high oxidation state, high electronegativity and weak polarizability.

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