Fractionated hydrosoluble copper indium sulfide quantum dots for solar cell sensitization

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Due to their interesting optical and electrical properties, quantum dots (QDs) have been subject of numerous scientific works worldwide and are considered promising materials for photovoltaic applications. QD solar cells are mainly focused on highly toxic cadmium and lead chalcogenides, raising questions concerning their future commercial applications due to health and environmental concerns. In this respect, development of "eco-friendly" quantum dots without heavy elements is of high importance. Ternary nanocrystals, such as $CuInS_2$, combine the classical advantages of QDs with non-toxicity and possibility to fine tune their properties in a larger range due to the wider choice of composition.[1] Typically, their synthesis is performed in organic phase and QDs are coated by long passivating ligands. For QD sensitized solar cells demonstrating the best photoconversion efficiency the QDs need to be transferred to water by ligand exchange, which adds an extra step to the fabrication procedure and can degrade the QD properties. Moreover, the use of organic solvents should be generally limited for ecological reasons. Therefore, it is important to develop syntheses of CIS QDs for photovoltaic applications directly in aqueous media.[2]

In this work water-soluble CIS quantum dots coated with mercaptopropionic acid (MPA) ligands were synthesized by a hydrothermal method. Several conditions have been tested to study the QDs formation mechanism. Using selective precipitation, three fractions of material were obtained and characterized using a variety of methods revealing considerably different compositions and optical properties (absorption, photoluminescence) and showing the importance of the fractionation of the reaction mixture. For the first time fractionated CIS QDs were applied for the sensitization of TiO_2 and ZnO substrates for use as photoanodes in quantum dot sensitized solar cells. The cells were fabricated using copper sulfide as counter-electrodes and polysulfide as electrolyte and characterized under simulated sunlight (Fig. and table 1). Various CIS fractions resulted in different photovoltaic behavior in cells due to the photocurrent generation by nanocrystals having slightly different sizes and composition but originating from the same synthesis. Application of thin passivation ZnS layer allowed for a considerable improvement of the solar cells efficiency due to the limitation of the recombination processes. The influence of the synthesis and fractionation conditions on eco-friendly QD sensitized solar cells performance will be discussed.

Fig. 1 Photoluminescence of fractionated CIS QDs.

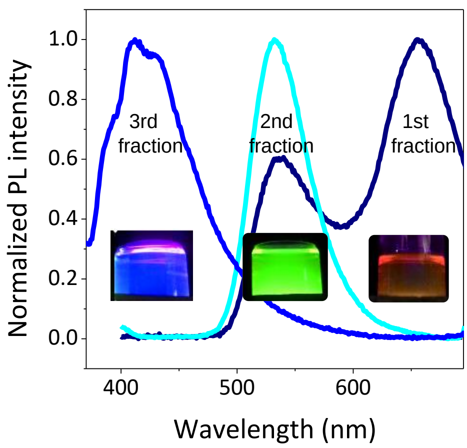

Table 1. Photovoltaic parameters of the fractionated QDs.

Sample	V_{oc} (V)	J_{sc} (mA/cm²)	FF (%)	η (%)
CIS 1st fraction/ZnS	0.51	8.18	57	**2,39**
CIS 2nd fraction/ZnS	0.52	9.18	61	**2,91**

1) D. Aldakov *et al.*, *J. Mater. Chem. C* **2013**, *1*, 3756-3776.
2) A. Raevskaya et al., *RSC Adv.*, **2016**, 6, 100145.