End-capping of low band gap conjugated polymer for metal-oxide nanoparticles surface modification

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In the field of polymer solar cells, the improvement of the bulk heterojunction (BHJ) in the active layer has been the topic of intensive research. [1] Among the possible electron donor materials in the BHJ, low band gap (LBG) conjugated polymer started to attract more attention because of their absorption within the solar emission, their number of delocalized π electrons and their smaller bandgap enhancing the power conversion efficiency. [2] One current problem is the bad stability of the BHJ due to aggregation of LBG or multi-phase morphology. [3] Hybrid solar cells using inorganic materials as acceptor material and conjugated polymers in the BHJ display a new trend to outperform organic electronic materials and to improve morphology and stability against oxygen and moisture in the active layer. [4] In addition to their ease of fabrication and low production costs, hybrid materials enhance interfaces with the optimization of charge injection, transport and recombination. [5]

We demonstrate an efficient strategy to anchor an end-functionalized low band gap polymer P(A-B) onto zinc oxide (ZnO) nanospheres to elaborate hybrid materials with tunable photophysical properties.

Fluorescence emission spectra of chloroform solutions of P(A-B)$_{(0)}$, grafted ZnO NPs, and a mixture composed of ZnO and P(A-B)$_{(0)}$ (weight ratio = 0,9075/0,0925)

The P(A-B) macromolecule was prepared *via* Stille coupling with a ternary reaction mixing monomer A, monomer B and an end-capper. [6] ^{1}H NMR and DOSY NMR spectra were performed to characterize the polymer. This polymer was then grafted onto ZnO nanospheres to create a macromolecular self-assembled monolayer (MSAM). This versatile technique introduces a new one pot strategy based on coupling reaction and could be applied to different metal oxide nanoparticles such as silicon, titanium or indium-tin oxide. The theoretical grafting density has been calculated and then determined, as well as polymer shell thickness *via* thermo gravimetric analysis and transmission electron microscopy. The optical properties of the hybrid material were ascertained by UV-visible absorption and fluorescence to show a specific quenching effect and to anticipate their potential applications in active layer of photovoltaic cells.

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