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n-type materials for solar cell devices: From Characterization to implementation in solar cells

Final Report

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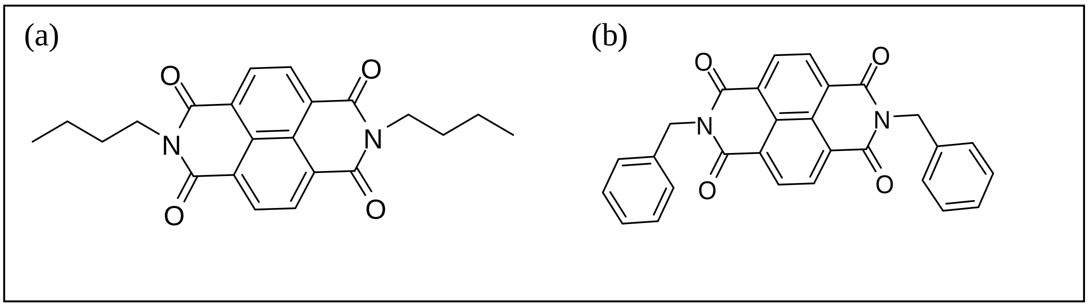
Purpose of the visit: to characterized by UV-visible (UV-vis), Photoluminescence (PL) spectroscopy and Atomic Force Microscopy (AFM) different mixtures of poly(3-hexylthiophene)(P3HT) and naphthalene diimide with different substituents namely, butyl-naphthalene diimide (Bu-NDI) and benzene-naphthalene diimide (Bn-NDI).

Work carried out during the visit: Based on the results obtained during my previous visit to LIOS (8-28.03.2010) both butyl-naphthalene diimide (Bu-NDI) and benzene-naphthalene diimide (Bn-NDI) can be viewed as n-type materials. The chemical structures of the materials are shown in Scheme 1. Thus, both materials were mixed with poly(3-hexylthiophene)(P3HT) in different ratios and the mixtures were analyzed by UV-visible (UV-vis) and Photoluminescence (PL) spectroscopy. Despite the optical and electrochemical properties of the materials, the morphology is a crucial parameter. Thus, Atomic Force Microscopy (AFM) was used to analyze the morphology of the different mixtures.



***Scheme 1**. Chemical structures of Bu-NDI (a) and Bn-NDI (b)*

For UV-Vis, Photoluminescence (PL) and Atomic Force Microscopy (AFM) measurements, mixtures of butyl naphthalene diimides (Bu-NDI) and benzene naphthalene diimides (Bn-NDI) with poly(3-hexylthiophene) (P3HT) with constant total concentration of 5 mg in 1 mL of chlorobenzene for each solution were prepared. In all the experiments different concentrations (80%, 60%, 50%, 40%, 20%) of P3HT in Bu-NDI and Bn-NDI were used. As a standards samples containing only pure NDIs or P3HT were used. Samples for UV-VIS, PL and AFM measurements were prepared by spin coating of different P3HT:NDI solution onto glass/ITO substrates.

The UV-vis absorption spectrum of P3HT is characterized by a broad absorption peak at 540 nm. From the UV-vis spectroscopy results, it can be said, that with increasing the concentration of the acceptor materials (both Bu-NDI and Bn-NDI) the absorption peak related to the P3HT decreases and a new feature related to the NDI derivates start to grow at approx. 340 nm.

PL measurements show a decrease in the emission peak of P3HT by increasing the concentration of both Bn-NDI and Bu-NDI. This experimental result might be a proof of charge transfer between the donor (P3HT) and acceptor materials (Bu-NDi and Bn-NDI). These experimental results open up the possibility of using mixtures of P3HT and the different naphthalene diimides as the active layer in organic solar cells (OSCs).

AFM images of mixtures of P3HT containing different concentration of the acceptor material (naphthalene diimide derivates) show a strong phase separation with increasing the concentration of the diimide derivates. This morphology is not yet the optimum one for the successfully use of these mixtures in a solar cell configuration.

Conclusions: From the experimental results UV-vis and PL spectroscopy, it can be said that both Bu-NDI and Bn-NDI can act as an acceptor materials together with P3HT as donor material in bulk heterojunction solar cells. However, the morphology of the resultant mixtures is not optimal and should be optimized by changing different parameters, e.g solvent.

Projected Publication: The results briefly summarized in this report will be complemented with the experimental results obtained in the previous visit of the applicant to LIOS in March and will result in a join manuscript.

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