Nanocomposites and nanomaterials

Effect of confinement on physical properties of P3HT chains in PMMA matrix

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Poly(3-hexylthiophene) (P3HT) is a promising polymer for application in organic photovoltaic (OPV) cells. The most known combination of P3HT and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) was invented in early 1990s [1,2] and remains a "classic landmark" for OPV cells. Arrangement of P3HT chains in the OPV structure has a great impact on the performance of the cell itself.

The goal of this work is to show how the changed arrangement of P3HT chains influences physical properties of P3HT aggregates such as electronic absorption spectrum, band gap, and photoluminescence quantum yield. In order to induce variation in mutual arrangement of the polymer chain, P3HT molecules were embedded into poly(methyl methacrylate) (PMMA) matrix to form a polymer composite. The PMMA matrix served to squeeze P3HT aggregates and to change their structure, respectively, under the action of hydrophobic forces. As a result, micron- and submicron-sized particles of P3HT were formed under certain conditions of preparation in PMMA matrix. The composite samples showed systematic changes in physical characteristics of P3HT aggregates. As the weight ratio of P3HT to PMMA decreased, the P3HT fraction demonstrated the red shift in band gap, the increase in ordering and the enhancement of quantum yield of photoluminescence.

The results are interpreted in terms of the changing intermolecular packing and reducing intramolecular torsional disorder. It is discussed the most contribution to the above changes comes from P3HT molecules at the interface of P3HT aggregate and PMMA environment.

- Morita S., Zakhidov A. A., Yoshino K. Doping effect of Buckminsterfullerene in conducting polymer — change of absorption spectrum and quenching of luminescence// Solid State Commun. -1992- 82, P. 249–252.
- 2. Saricifici N. S., Smilowitz L., Heeger A. J., Wudl F. Semiconducting polymers (as donors) and Buckminsterfullerene (as acceptor) photoinduced electron-transfer and heterojunction devices// Synth. Met. -1993.- **59**, P. 333–352.