Thermodynamic Effects in Morphological Evolution of Polymer-Fullerene Nanocomposites for Photovoltaic Applications

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Polymer based photovoltaic devices promise solar technologies that are inexpensive enough to be widely exploited and therefore provide a significant fraction of the future energy needs. There are many promising polymer-fullerene mixtures that are promising materials candidates for achieving high performance devices, but their exploitation requires and improved understanding of their structure-property relationships. Of particular relevance is the phase behavior of the mixtures.

The phase behavior of donor-acceptor materials for photovoltaic applications is of key importance [1,2]: i) to gain a fundamental understanding and control of morphology development in the donor-acceptor blends; ii) to appropriately choose the operating window for thermal annealing; iii) to understand the long-term stability of the blended film morphology and consequently of the photovoltaic performance of the corresponding solar cells.

In this work the phase behavior of polymer-fullerene mixtures is being studied using Differential Scanning Calorimetry (DSC), Wide-Angle X-Ray Scattering (WAXS), Small-Angle Neutron Scattering (SANS) and theoretical *ab initio* Density Functional Theory (DFT) calculations.

References:

[1] J. Zhao, A. Swinnen, G. V. Assche, J. Manca, D. Vanderzande, B. Van Mele, Phase Diagram of P3HT/PCBM Blends and Its Implication for the Stability of Morphology, J. Phys. Chem. B, **113**, 1587 (2009)

[2] J. Y. Kim, C. D. Frisbie, Correlation of Phase Behavior and Charge Transport in Conjugated Polymer/Fullerene Blends, J. Phys. Chem. C, **112**, 17726 (2008)