Understanding the microstructure of polymer-metaloxide hybrid interfaces

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Polymer metaloxide hybrids have emerged as promising systems for photovoltaics combining the formability of polymers and the good transport properties and thermal stability of the inorganic component. A strong link of the polymer (where light is absorbed) to the inorganic substrate (where electrons are accepted) and a crystalline microstructure of the polymer at the interface are necessary to give rise to an efficient photoconversion. Accordingly, the theoretical understanding of the interface morphology at the atomic scale is of great relevance to improve the properties of such hybrid materials.
We adopt a hierachic combination of model potential and first-principles atomistic methods to generate realistic models of interface between poly3hexylthiophene (P3HT) and nanostructured metaloxides such as titanium dioxide (TiO2) and zinc oxide (ZnO). This work is part of a research effort (Seed Project "POLYPHEMO" [1]) aimed at modeling polymer based hybrid nanomaterials for photovoltaics.
We provide evidence that the polymer organization at the interface (both in vacuo or in presence of typical solvents such as tetrahydrofuran) strongly affects the properties of the system. It is found that the polymer adhesion depends on the curvature at the nanoscale and on the local charge of the metaloxide [1]. Furthermore, the polymer assembling [2] at the interface critically affects the transport properties[3]. In particular P3HT tends to be disordered rather than crystalline at the interface with ZnO. The implications on the local transport properties and photoconversion efficiency are discussed.
Wrapping phenomena of P3HT on carbon nanotubes [4] and ZnO nanoneedles and their effects on the electronic properties of the hybrids are discussed as well.
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