Nanoscale morphology at the dielectric/semiconductor interface in organic field-effect transistors

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Organic molecules and polymers represent nowadays an attractive class of materials for the development of novel efficient, multifunctional and bio-compatible electronic devices, e.g. organic field-effect transistors (OFETs). Despite the increase in the industrial relevance of these devices, however, many aspects of their working mechanism are still unclear. Namely, a crucial issue in their fabrication is the nanoscale morhology at the interface between different layer, which affects greatly their performances. In this work, the nanoscale morphology at the dielectric/semiconductor interface in organic field-effect transistors (OFETs) is investigated.

Firstly, the correlation between the morphology of polymeric materials at the nanoscale and charge carrier mobility in OFETs is studied by an integrated approach based on atomistic molecular dynamics (MD) and kinetic Monte Carlo (KMC) simulations. The morphology of the gate dielectric obtained with MD simulations is used to define a simple model for KMC calculations of charge carrier mobility in a generic overlying semiconductor material. Our results indicate a tight correlation between processing and thermal treatments of the gate dielectric material and device performance.

Moreover, further MD simulations are performed to investigate the polymorphism and the morphology of a prototypical n-type organic semiconductor based on the perylene diimide core, PTCDI-C13, at the interface with the gate dielectric material. Starting from the atomistic simulations of molecular packing and polymorphism in 2-dimensional aggregates, advanced computational techniques are applied to the simulation of growth of complex morphologies at the dielectric/semiconductor interface. Our results are consistent with a Stranski-Krastanov growth of the PTCDI-C13 on PMMA, as evidenced in experiments. Namely, MD simulations allow the detailed analysis, with atomistic resolution, of processes related to the formation of ordered aggregates, nanocrystalline structures and grain boundaries, in the growth of the organic semiconductor layer at the interface with the dielectric material.