Materials-Scale Implications of Solvent and Temperature on [6,6]-Phenyl-C61-butyric Acid Methyl Ester (PCBM): A Theoretical Perspective

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Abstract

The ability to detail how molecules pack in the bulk and at the various materials interfaces in the active layer of an organic solar cell is important to further understanding overall device performance. Here, [6,6]-phenyl-C-61-butyric acid methyl ester (PCBM), a preferred electron-acceptor material in organic solar cells, is studied through molecular dynamics (MD) simulations; the goal is to examine the effects of temperature and trace solvents on the packing and morphological features of bulk PCBM. Solubility (miscibility) parameters, melting and order-disorder transitions, surface energies, and orientational distributions as a function of different starting configurations are discussed. On the basis of the derived morphologies, electronic structure calculations and a kinetic Monte Carlo approach are combined to evaluate the parameters impacting electron mobility in crystalline and amorphous PCBM structures.

Keywords

Author Keywords: organic photovoltaics; fullerenes; phase transitions; annealing; electron transport

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