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Self-assembly of Poly(3-hexylthiophene) with nanostructured inorganic semiconductors for applications in photovoltaics: a computational study MARCO BERNARDI, JEFFREY C. GROSSMAN, MIT — A number of functional materials based on blends of polythiophene derivatives and inorganic materials have been investigated in recent years for optoelectronic applications. For example, blends of Poly(3-hexylthiophene) (P3HT) and C60 are particularly efficient as donor-acceptor systems for bulk heterojunction organic photovoltaic solar cells due to high interfacial area and ultrafast photoinduced electron transfer. The increased availability of novel forms of nanostructured semiconductors with different surface functionalizations motivates the investigation of self-assembled P3HT with quantum dots, nanowires, thin films and other nanostructured semiconductors for applications in photovoltaics. Results based on classical molecular dynamics simulations of the self-assembly of P3HT with some of these materials will be presented. Density functional theory calculations are utilized to predict the dependence of the electronic structure of the self-assembled materials on interfacial surface chemistry and nanoscale curvature effects.

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