

Mesoscopic modeling of liquid crystalline mesophases in semiconducting polymers

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Soluble semiconducting polymers frequently form partially-ordered mesophases [1,2]. These mesophases “bridge” the two extremities of the order-disorder scale corresponding to (poly)crystalline and amorphous morphologies. Technologically, partially-ordered mesophases are important because they can lead to improved optoelectronic properties [1,2]. For basic polymer physics, these mesophases present significant interest because they enable systematic generation of different degrees of order. This feature can help, e.g. understanding phenomena during polymer crystallization.

Here we focus on a special class of partially ordered structures: liquid crystalline mesophases. To model these mesophases we develop a computationally-efficient simulation strategy [3-5]. The approach is based on coarse-grained descriptions of polymer architecture and “soft” anisotropic non-bonded potentials. Their phenomenological definition takes into account generic symmetries of molecular order in the studied mesophase. We demonstrate that the approach can describe a sequence of mesophases with increasing degree of order: from uniaxial nematic to lamellar-like, smectic [6], morphologies. For uniaxial nematics, the approach reduces to a compressible Maier-Saupe model. Using uniaxial nematics as an example, we discuss the problem of materials-specific parameterization of phenomenological potentials from experimental data [7]. Next we focus on smectic mesophases and discuss their molecular organization. The lamellar order is characterized by various quantifiers, such as scattering patterns that can be compared with experimental GIWAXS. We demonstrate that our smectic mesophases match morphologies that have been experimentally observed in P3HT [8]. We conclude with an outlook highlighting some directions for further methodological developments and applications.

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