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Frank elastic constants in LC mesophases of polymeric semiconductors[1] PATRICK GEMUENDEN, KURT KREMER, KOSTAS CH. DAOULAS, Max Planck Institute for Polymer Research, Germany — Liquid crystalline (LC) mesophases of polymeric semiconductors [1], e.g. poly(alkylthiophenes), can facilitate processing to obtain morphologies with improved properties. We develop a particle-based modeling approach to study nematic mesophases of such systems. The method uses soft, directional interactions [2] and is inspired by field theoretical approaches to LCs [3]. It enables us to generate large morphologies and calculate Frank elastic constants (FC). Besides interesting theoretical questions related to the behavior of FCs in polymer nematics, they are important when linking particle-based with continuum media descriptions of LCs. We calculate FC related to bend, splay and twist deformations from the fluctuation spectra of the local nematic director. The magnitudes of FC measured in the simulations agree with those reported in experiments on polymer nematics. We discuss their dependence on system parameters, e.g. chain length, and we compare with predictions by analytical field theory [4].

[1] Ho et al., Macromolecules 43, 7895 (2010)
[2] Gemünden et al. Macromolecules 46, 5762 (2013)
[3] Pryamitsyn & Ganesan, J. Chem. Phys. 120, 5824 (2004)
[4] Le Doussal & Nelson, Europhys. Lett. 15, 161 (1991)

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