Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Tuesday,
2nd July 2019

at: **5.15pm**

VDP 4 1.27,
Von-Danckelmann-Platz 4
06120 Halle

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"Investigating partially-ordered mesophases of semi-conducting polymers with mesoscopic models"

The rich phase behavior of soluble semiconducting polymers makes them interesting for basic polymer physics, allowing one to access partially-ordered states ─ microstructures located on the order-disorder scale between the two extremities set by (poly)crystalline and amorphous morphologies. Studying microstructures with varying degree of order can facilitate, e.g. understanding of polymer crystallization phenomena.
Technologically, partially-ordered phases are interesting because of their relevance to new-generation materials with improved charge-transport properties [1].
We present a computationally-efficient simulation strategy [2,3] for investigating the molecular organization in partially-ordered mesophases. Semiconducting polymers are described by chains of coarse-grained monomers; each of these monomers represents (at least) one atomistic repeat unit. Despite this drastic coarse-graining, atomistic-scale anisotropicities caused, e.g. by pi-interactions, are captured thanks to non-bonded anisotropic potentials motivated by generic symmetries of molecular order. It will be demonstrated that the approach can describe a broad spectrum of morphologies, including amorphous, nematic, and lamellar-like, sanidic, mesophases. We will extensively discuss the molecular organization of these morphologies, focusing on sanidic mesophases. Several quantifiers will be used to characterize lamellar order, including scattering patterns that can be compared with experimental GIWAXS. We will demonstrate that our sanidic mesophases match morphologies that have been experimentally observed in P3HT [4]. We will conclude with an outlook for applying our modeling approach to problems relevant for polymer crystallization.

[1] Noriega R., Rivnay J., Vandewal K., Koch F.P.V., Stingelin N., Smith P., Toney M.F., and Salleo A., Nat. Mater. 2013, 12, 1038 [2] Gemünden P., Poelking C., Kremer K., Andrienko D., and Daoulas K.C., Macromolecules 2013, 46, 5762 [3] Greco C., Melnyk A., Kremer K., Andrienko D., and Daoulas K.C., Macromolecules 2019, 52, 968 [4] Wu Z., Petzold A., Henze T., Thurn-Albrecht T., Lohwasser R.H., Sommer M., and Thelakkat M., Macromolecules 2010, 43, 4646