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Thermodynamics of polymer nematics described with a worm-like chain model: particle-based simulations and SCF theory calculations
CRISTINA GRECO, Max Planck Institute for Polymer Research, Mainz, Germany , YING YIANG, School of Chemistry and Environment, Center of Soft Matter Physics and Its Applications, BeiHang University, Beijing, China, KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany , JEFF CHEN, Department of Physics and Astronomy, University of Waterloo, Canada, KOSTAS DAOULAS, Max Planck Institute for Polymer Research, Mainz, Germany — Polymer liquid crystals, apart from traditional applications as high strength materials, are important for new technologies, e.g. Organic Electronics. Their studies often invoke mesoscale models, parameterized to reproduce thermodynamic properties of the real material. Such top-down strategies require advanced simulation techniques, predicting accurately the thermodynamics of mesoscale models as a function of characteristic features and parameters. Here a recently developed model [1] describing nematic polymers as worm-like chains interacting with soft directional potentials is considered. We present a special thermodynamic integration scheme delivering free energies in particle-based Monte Carlo simulations of this model, avoiding thermodynamic singularities. Conformational and structural properties, as well as Helmholtz free energies are reported as a function of interaction strength. They are compared with state-of-art SCF calculations [2] invoking a continuum analog of the same model, demonstrating the role of liquid-packing and fluctuations. [1] P. Gemnden and K.Ch. Daoulas, Soft Matter 2015, 11, 532; [2] Y. Jiang and J.Z.Y. Chen, Macromolecules 2010, 43, 10668.

Kostas Daoulas
Max Planck Institute for Polymer Research

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