pyPRISM: A Computational Tool for Liquid-State Theory Calculations of Macromolecular Materials

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Polymer Reference Interaction Site Model (PRISM) theory describes the equilibrium spatial-correlations of liquid-like polymer systems including melts, blends, solutions, block copolymers, ionomers, polyelectrolytes, liquid crystal forming polymers and nanocomposites. Using PRISM theory, one can calculate thermodynamic (second virial coefficient, χ interaction parameters, potential of mean force) and structural (pair correlation functions, structure factor) information for these macromolecular materials.

Here, we present a Python-based, open-source framework, pyPRISM, for conducting PRISM theory calculations. This framework aims to simplify PRISM-based studies by providing a user-friendly scripting interface for setting up and numerically solving the PRISM equations. pyPRISM also provides data structures, functions, and classes that streamline PRISM calculations, allowing pyPRISM to be extended for use in other tasks such as the coarse-graining of atomistic simulation force-fields or the modeling of experimental scattering data. The goal of providing this framework is to reduce the barrier to correctly and appropriately using PRISM theory and to provide a platform for rapid calculations of the structure and thermodynamics of polymeric fluids and nanocomposites.