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Overlap free energy of polymers under cylindrical confinement[1]
JAMES POLSON, AIDAN TREMBLETT, DEANNA KERRY, Univ of Prince Edward Island — Polymers subject to cylindrical confinement can experience intramolecular overlap due to internal folding or intermolecular overlap with other polymers, and the free energy cost of chain overlap drives single-chain unfolding or multi-chain segregation, respectively. Theoretical treatments of such dynamical processes often employ analytical approximations of the conformational free energy. In this study, Monte Carlo simulations are used to measure the overlap free energy of polymers subject to cylindrical confinement. The calculated free energy functions are used to test the predictions of scaling theories and quantify the finite-size effects. We calculate the conformational free energy of a single folded polymer as a function of the position of the fold along the tube for both flexible and semi-flexible hard-sphere chains. We also examine the cases of arm retraction in star polymers and the segregation of ring polymers under cylindrical confinement. The scaling of the free energy functions with chain length and stiffness, as well as confinement diameter, are generally consistent with theoretical predictions, though appreciable deviations due to finite-size effects persist for chains up to N=500 monomers.

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