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Surface induced alignment for semiflexible polymers WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State University — The interfacial structure of semiflexible polymers can largely affect the overall performance of applications, such as organic electronics. Due to backbone stiffness, semiflexible polymers, including conjugated polymers, tend to align parallel to an impenetrable surface. The segmental alignment near the wall creates a quadrupolar aligning field, which can interact with the polymer backbones and enhance the chain alignment. In the present work, we combine molecular dynamic (MD) simulations and a lattice version of self-consistent field theory (SCFT) to investigate the surface induced alignment for semiflexible polymers. Using MD simulations of bead-spring chains, we demonstrate that the thickness of the aligned layer is about a persistence length L_p for semiflexible polymers in the isotropic phase. Using the SCFT lattice model, we predict that the amplitude and range of the alignment increase with increasing nematic coupling, quantified by the nematic coupling constant α. The impenetrable surface acts as a perturbation on the chain alignment, and the nematic coupling α amplifies the perturbation. By comparing the SCFT results for chains near an impenetrable surface to MD simulations, we can also qualitatively estimate α for semiflexible polymers.

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