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Two-dimensional semiflexible polymers under external fields

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The non-equilibrium structural and dynamical properties of semiflexible polymers confined to two dimensions are investigated by molecular dynamics simulations. Three different scenarios are considered: The force-extension relation of tethered polymers, the relaxation of an initially stretched semiflexible polymer, and semiflexible polymers under shear flow. We find quantitative agreement with theoretical predictions for the force-extension relation and the time dependence of the entropically contracting polymer. The semiflexible polymers under shear flow exhibit significant conformational changes at large shear rates, where less stiff polymers are extended by the flow, whereas rather stiff polymers are contracted. In addition, the polymers are aligned by the flow, thereby the two-dimensional semiflexible polymers behave similarly to flexible polymers in three dimensions. The tumbling times display a power-law dependence at high shear rate rates with an exponent comparable to the one of flexible polymers in three-dimensional systems.

References

[1] A. Lamura, R.G. Winkler: *Semiflexible polymers under external fields confined to two dimensions*. J. Chem. Phys. **137**, 244909 (2012)