سمینار هفتگی ماده چگال نرم

# Simulating wet active polymers by multiparticle collision dynamics

## Abstract

In this talk I'm going to talk about an article based on simulating wet active polymers. The conformational and dynamical properties of active Brownian polymers embedded in a fluid depend on the nature of the driving mechanism, e.g., self-propulsion or external actuation of the monomers. Implementations of self-propelled and actuated active Brownian polymers in a multiparticle collision dynamics (MPC) fluid are presented, which capture the distinct differences between the two driving mechanisms. The active force-free nature of self-propelled monomers requires adaptations of the MPC simulation scheme, with its streaming and collision steps, where the monomer self-propulsion velocity has to be omitted in the collision step. Comparison of MPC simulation results for active polymers in dilute solution with results of Brownian dynamics simulations accounting for hydrodynamics via the Rotne-Prager-Yamakawa tensor confirm the suitability of the implementation. The polymer conformational and dynamical properties are analyzed by the static and dynamic structure factor, and the scaling behavior of the latter with respect to the wave-number and time dependence are discussed. The dynamic structure factor displays various activity-induced temporal regimes, depending on the considered wave number, which reflect the persistent diffusive motion of the whole polymer at small wave numbers, and the activity-enhanced internal dynamics at large wave numbers. The obtained simulation results are compared with theoretical predictions.

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