Globule-like conformation and enhanced diffusion of active polymers

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We study the dynamics and conformation of polymers composed by active monomers. By means of Brownian dynamics simulations we show that when the direction of the self-propulsion of each monomer is aligned with the backbone, the polymer undergoes a coil-to-globule-like transition, highlighted by a marked change of the scaling exponent of the gyration radius.

Concurrently, the diffusion coefficient of the center of mass of the polymer becomes essentially independent of the polymer size for sufficiently long polymers or large magnitudes of the self-propulsion. These effects are reduced when the self-propulsion of the monomers is not bound to be tangent to the backbone of the polymer.

Our results, rationalized by a minimal stochastic model, open new routes for activity-controlled polymer and, possibly, for a new generation of polymer-based drug carriers [1].

[1] V. Bianco, E. Locatelli, and P. Malgaretti, Globule-like conformation and enhanced diffusion of active polymers, arXiv: 1805.08879.