Single-Chain Polymer Nanoparticles: Models for Intrinsically Disordered Proteins and Soft Glass-Formers

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Single chain nanoparticles (SCNPs) represent an emergent and promising class of synthetic nano-objects. By means of large-scale computer simulations and small-angle neutron scattering (SANS), we design and investigate different synthesis routes, leading to SCNPs with specific conformations and structure and eventually distinguishing properties in solution. On one hand the analysis of the conformational properties of sparse SCNPs synthesized in good solvent reveals that these synthetic nano-objects share basic ingredients with intrinsically disordered proteins (IDPs), as topological polydispersity, generally sparse conformations, and locally compact domains. Unlike in the case of linear macromolecules, crowding leads to collapsed conformations of SCNPs resembling those of crumpled globules at volume fractions (about 30 %) that are characteristic of crowding in cellular environments. Our results for SCNPs — a model system free of specific interactions — propose a general scenario for the effect of steric crowding on IDPs. On the other hand, dense solutions of globular SCNPs obtained via solvent-assisted routes show soft caging, reentrant diffusivity and weak dynamic heterogeneity. Quantitative differences depend on the specific nanoparticle degree of compressibility, i.e. on the specific synthesis route adopted, as well as on the intrinsic topological polydispersity. This new class of soft glass-forming systems opens up the possibility of getting insight into the mechanisms of diffusion in crowded environments (like globular proteins in cells or porous media) as well as to draw new strategies for tailoring rheological properties of polymer based nanomaterials.