Synthesis routes and crowding effects on single-chain polymeric nanoparticles: Combining simulations and small-angle neutron and X-ray scattering

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Polymeric single-chain nanoparticles (SCNPs) are an emergent class of soft nano-objects of molecular size of 5-20 nm, resulting from the purely intramolecular cross-linking of the reactional functional groups of single polymer precursors. A growing interest is being devoted in recent years to develop a SCNP-based technology with multiple applications in catalysis, nanomedicine, or rheology, amongst others. To this end, we need good control over the size and shape of SCNPs, as well as a deeper understanding of their behaviour in complex situations as macromolecular crowding. By means of computer simulations of coarse-grained models and validation by small-angle neutron and X-ray scattering, we design and investigate different protocols leading to SCNPs with specific structures and different properties in solution.

The analysis of the conformations of SCNPs synthesized in good solvent reveals that they share basic ingredients with intrinsically disordered proteins (IDPs), as topological polydispersity, sparse conformations, and compact local domains [1]. Unlike in the case of linear macromolecules, crowding leads to collapsed conformations of SCNPs resembling those of crumpled globules [1,2], at volume fractions (about 30%) that are characteristic of crowding in cellular environments. This result is apparently universal and independent of the architecture of the polymers crowding the environment of the SCNP [2]. Our results for SCNPs - a model system free of specific interactions - propose a general scenario for the effect of steric crowding on IDPs.

[1] A.J. Moreno, F. Lo Verso, A. Arbe, J.A. Pomposo, J. Colmenero, Journal of Physical Chemistry Letters **7**, 838 (2016)

[2] M. González-Burgos, A. Arbe, A.J. Moreno, J.A. Pomposo, A. Radulescu, J. Colmenero, Macromolecules **51**, 1573 (2018)

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