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Structure of Single-Chain Nanoparticles Under Crowding Conditions: A Random Phase Approximation Approach

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Macromolecules in biological systems *in vivo* are in the cell's crowded environment, which can modify biological function through changes in the structural conformation with respect to diluted conditions. The structural characterization in crowded media is challenging given the high concentration and the intrinsic complexity in these samples. To address the topological effects, we use model single-chain nanoparticles (SCNPs) —single-stranded polymers partially collapsed via intramolecular bonding. Neutron scattering is the best method to probe the structure of small concentrations of labeled chains in the presence of large concentrations of other species. Yet, at high concentration, even mild polymer-solvent interactions contribute to the scattering. To account for such effects, the Random Phase Approximation (RPA) formalism applies.
Here, we study with small angle neutron scattering (SANS) the conformation of poly methyl methacrylate (PMMA)-based SCNPs and linear precursors in dilute and in crowding with linear PMMA chains in deuterated dimethylformamide (DMF). The SANS profiles were analyzed in terms of a three-component (probe, crowder and solvent) RPA model to consider the polymer-solvent interactions. The presence of the crowder produces a size reduction on the probes. The Flory-Huggins interaction parameter varies with the sample composition indicating that in the dilute regime DMF is a good solvent for PMMA while in crowded conditions the polymer becomes less soluble.

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