Structure and Dynamics of Single-Chain Nano-Particles in Solution

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Single Chain Nano-Particles (SCNPs) are polymeric soft nano-objects consisting of unimacromolecular chains collapsed to a certain degree by means of intramolecular bonding. The usual techniques for SCNPs formation result in sparse, non-globular morphologies in solution [1] that are very similar to those displayed by bio-macromolecules, in particular by intrinsically disordered proteins (IDPs) [2]. IDPs and SCNPs are intrinsically polydisperse both in size and topology [3]. The similarities between SCNPs and IDPs suggest using SCNPs as model to mimic bio-macromolecules in different environments and situations. The ultimate goal of biomolecular studies is to understand the behavior of these entities in realistic situations (cellular environment), where macromolecular solutions are highly concentrated. The effective nano-confined induced by crowders can dramatically modify biological function, through changes in the conformation and dynamics of the macromolecules respect to diluted in vitro conditions [4]. We could thus exploit the analogies found between SCNPs and IDPs to address the essential question of the change of the properties of biomacromolecules in increasingly crowded environments.

We present an investigation, by combining small-angle neutron scattering (SANS) and coarse-grained molecular dynamics (MD) simulations, on the conformational properties of single-chain nano-particles (SCNPs) in crowded macromolecular solutions. By using linear chains as crowders, SANS shows a crossover from almost unperturbed SCNPs conformations in dilute conditions toward a continuous collapse of the macromolecule with increasing crowding. This collapse starts when the total concentration of the solution reaches the value of the overlap concentration of the pure SCNPs solutions. MD-simulations prove the generalizability of these experimental findings and extend them to the case when the SCNPs themselves are used as crowders -a situation which in real systems leads to unavoidable formation of aggregates, as shown here by SANS and DLS. In addition, we have investigated the dynamics of SCNPs in dilute solution by means of Neutron Spin Echo. The dynamic structure factor reveals a large impact of internal crosslink on the macromolecular mobility manifested as a high internal friction [5]. This is another striking resemblance with intrinsically disordered proteins [6].