[Talk 9] Polymer looping in crowded media: effects of volume fraction and size of crowder

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The cell is highly crowded with various macromolecules whose volume fraction can reach up to 30-35 %, therefore molecules in the cell behave in a radically different way than those in dilute solutions. Here we study the looping dynamics of polymer chains, a fundamental process in biology, in the presence of molecular crowding by using Langevin dynamics simulations. From the analysis of the looping probabilities of end-monomers and the looping-unlooping rates, we find that the small crowders (size chain monomer) typically $\simeq$ slow down the chain dynamics but with bigger crowders (size $\simeq$ chain gyration radius), the looping kinetics can be facilitated. We analyze the effects of the molecular crowding in terms of the excluded effects and the increase of viscosity. We find that for small crowders the effect of an increased viscosity dominates, while for bigger crowders the confinement (caging) effects prevail. The tradeoff between two effects can thus result in the impediment or facilitation of the looping, depending on the size of crowders. We discuss our results in connection with recent experiments on DNA hairpin formation in the presence of crowding molecules.

[1] J. Shin, A. G. Cherstvy, and R. Metlzer, Soft Matt.11, 472 (2015).