

Computational studies on the temperature-induced transition in PNnPAm hydrogels.

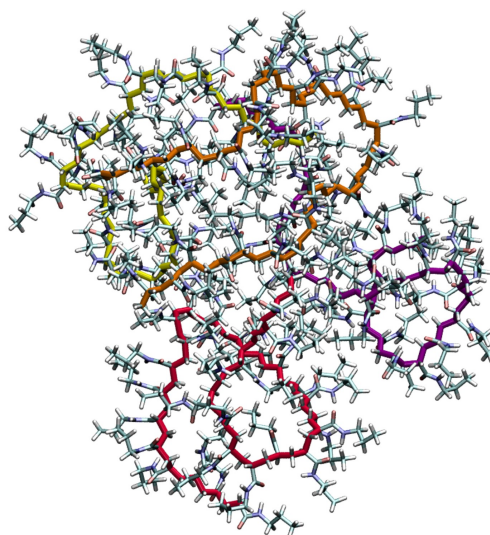
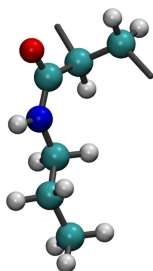
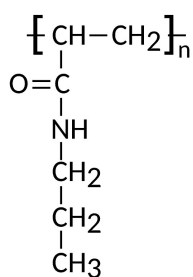
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Abstract: *N*-substituted acrylamide-based polymers are widely studied thermoresponsive polymers [1]. In particular, poly(*N*-*n*-propylacrylamide) (PNnPAm) exhibits a unique and sharp volume phase transition in aqueous solution, in contrast to poly(*N*-isopropylacrylamide) [2]. In this work, we carried out all-atom molecular dynamics simulations of single- and multiple-oligomers of PNnPAm with 32 repeating units solutions in water. Systems with one and four oligomers were investigated for two different temperatures, 280 and 340 K, below and above the LCST. Our analysis suggests that systems with multiple-oligomers form aggregates and assemble as a cluster, forming a physical gel at higher temperature [3]. Radius of gyration, inter-chain distances and number of contacts between chains, display all the temperature-dependent signature of the structural changes of PnnPAm.



(a)

(b)

(c)

Figure 1: (a) A schematic of a NnPAm monomer, (b) a snapshot of a NnPAm monomer and (c) snapshot of four PNnPAm chains at the end of 100 ns above the LCST (340 K).

Key-words: poly(*N*-isopropylacrylamide), PNnPAm, LCST, hydrogels.



XIX SBQT

Simpósio Brasileiro de Química Teórica 2017

12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

References:

- [1] T. E. de Oliveira, D. Mukherji, K. Kremer, P. A. Netz, J. Chem. Phys., 146, 034904 (2017).
- [2] B. Wedel, Y. Hertle, O. Wrede, J. Bookhold, and T. Hellweg, Polymers 8, 162 (2016).
- [3] T. E. de Oliveira *et al.* *to be submitted*, (2017).