

Further investigations into conformational transitions in a lattice model of three-component mixtures of solvent, amphiphile and soluble polymers

D.E. Jennings, Yu.A. Kuznetsov, E.G. Timoshenko, K.A. Dawson

Theory Group, Centre for Soft Condensed Matter and Biomaterials, Department of Chemistry, University College Dublin, Dublin 4, Ireland

Summary

We study the phase diagram of polymer-amphiphile-solvent mixtures in the dilute polymer limit. We investigate the effect of the polymer chain length, the strength of the amphiphilic interactions and the concentration of the amphiphil. on the type of structures formed. We have carried out extensive calculations for a variety of chain lengths, N , for a range of values of the effective three-body interaction constant.

In the almost pure solvent regime, the critical point corresponding to the coil-to-globule collapse transition decreases with increasing N . At higher amphiphile concentrations, the polymer collapses to a "layered" structure first and then to a globule. This collapse transition increases with increasing N as there are more favourable (m_{as}) and unfavourable (m_{am}) interactions stabilising the polymer-amphiphile structures. We also find that as N increases the transitions become sharper, the phenomena become more pronounced and the stability of the polymer-amphiphile layered structures increases.

Our overall conclusion is that it is feasible to study a polymer-amphiphile-water lattice model using a combination of Monte Carlo moves that sample a wide variety of configuration space. In particular we have noted that reptations are helpful for dilute polymer-amphiphile solutions, but essential for more dense amphiphile regimes. We have also noted that even with a minimal set of interactions, albeit consistent with the most elementary properties of amphiphiles and polymers, a non-trivial phase diagram emerges.

These results are in qualitative agreement with theoretical and experimental results.

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