Abstract

This dissertation presents an overview of our computer simulation studies of the conformational behaviour
of amphiphilic polymers. In the studies we showed that the polymers form a variety of self-organised structures at a single molecule level. These include the pearl-necklace structure, spherical and cylindrical intramolecular micelles and bundles. From the simulations we were able to obtain a deeper insight into the behaviour of amphiphilic polymers and conditions under which the above-mentioned structures are formed. Some of the results were compared to experimental or theoretical studies of similar polymers.
In some cases the simulations confirmed earlier interpretations which were based on analogy or intuition.
In other cases they revealed new phenomena which had not been considered before.