

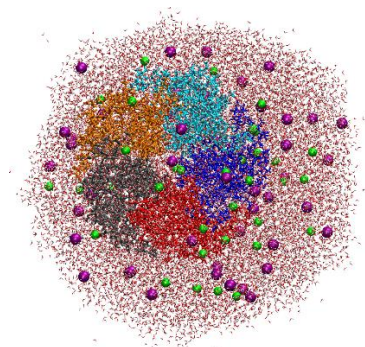
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Assembly of macromolecules in droplets

The droplet environment is distinct relative to the bulk analogue. A droplet is characterized by large surface to volume ratio and provides a confining environment. As a result, chemical reactions and assembly in droplets show different mechanisms, rates and equilibrium constants. In this project the assembly of linear and compact macromolecules in droplets will be studied.



During the course of the project the student(s) will learn state-of-the-art molecular modelling software packages (NAMD and VMD), molecular dynamics and Monte Carlo methods. Knowledge of a programming language such as Python, or C++ or C is a desirable skill but not necessary as long as the student is willing to dedicate the time to learn a programming language.

References

1. Kwan, V., Malevanets, A. and Consta, S., 2019. Where do the ions reside in a highly charged droplet?. *The Journal of Physical Chemistry A*, 123(43), pp.9298-9310.
2. Kwan, V. and Consta, S., 2020. Bridging electrostatic properties between nanoscopic and microscopic highly charged droplets. *Chemical Physics Letters*, p.137238.