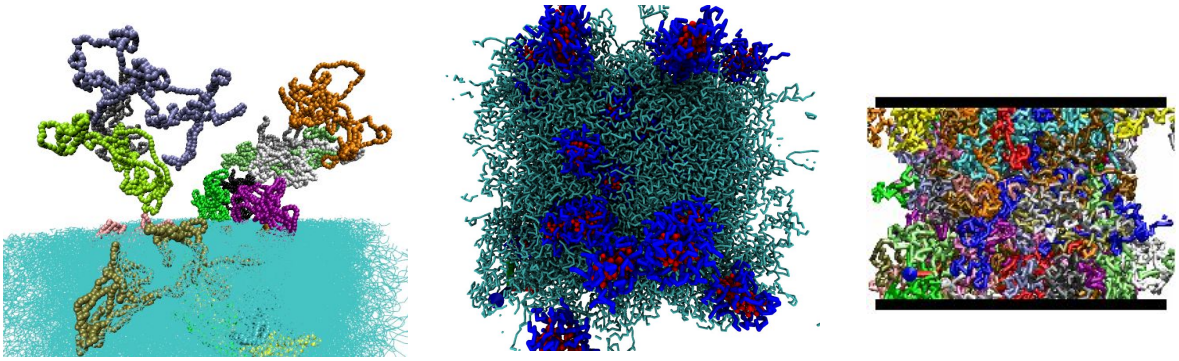
Computational study of polymer dynamics in melts of different architectures

DIRECTEUR DE THÈSE : HENDRIK MEYER
EQUIPE THEORIE ET SIMULATION DES POLYMERES
INSTITUT CHARLES SADRON, CNRS, 23, RUE DU LOESS, 67034 STRASBOURG
TEL : 03 88 41 40 32 ; E-MAIL : HENDRIK.MEYER@ICS-CNRS.UNISTRA.FR

Polymers have fascinating properties because of their broad spectrum of internal relaxation modes. In a multichain system as a polymer melt, the chains couple in addition to each other. Contrary to textbook knowledge, we have recently shown that hydrodynamic interactions are not immediately screened in polymer melts, and that their combination with the viscoelastic properties of the melt can explain different regimes of anomalous center-of-mass motion of the chain [1,2]. However, the theory could be solved exactly only for unentangled chains. The aim of this project is to implement a numerical framework to test the theory for melts of complex polymer architectures: rings or branched polymers which have very different viscoelastic properties from linear melts. The structural and viscoelastic properties have to be obtained from computer simulations which then serve as input for a numerical solution to predict the diffusion of the chains. The work could be extended to analyse confined melts [3] or mixtures with nanoparticles.



The candidate should have a good background in statistical physics and the taste of working with the computer as the main tool. Some knowledge of programming with C or Python is expected. Coarse-grained molecular dynamics simulations will be performed with the LAMMPS code, but the analysis will need programming of new tools.

[1] J. Farago, H. Meyer, and A.N. Semenov; A*nomalous Diffusion of a Polymer Chain in an Unentangled Melt* Phys. Rev. Lett. **107** (2011) 178301. J. Farago, H. Meyer, J. Baschnagel, and A.N. Semenov; *Mode-coupling approach to polymer diffusion in an unentangled melt: II. The effect of viscoelastic hydrodynamic interactions,* Phys. Rev. E **85** (2012) 051807.
[2] A.N. Semenov and H. Meyer; *Anomalous diffusion in polymer monolayers*, Soft Matter **9** (2013) 4249.
[3] H. Meyer, T. Kreer, A. Cavallo, J.P. Wittmer, and J. Baschnagel; *On the Dynamics and Disentanglement in Thin and Two-Dimensional Polymer Films*, Eur. Phys. J. Special Topics **141** (2007) 167. Nam-Kyung Lee, D. Diddens, H. Meyer, and A. Johner; *Local chain segregation and entanglements in a confined polymer melt*, Phys. Rev. Lett. **118** (2017) 067802.