Prof. Jean-Paul RYCKAERT
Université Libre de Bruxelles

Simulation at a mesoscopic level of diffusion-limited binding of proteins on living filaments.

In living filaments like actin and tubulin and also in some conventional biological semi-flexible molecules like DNA, the binding kinetics of single proteins on specific sites of the semi-flexible chain is a problem of high relevance related to the general class of diffusion-limited reactions. Theoretical developments combining the Smolukowcki approach for the kinetics and filament internal dynamics predictions have been reported on some general aspects of the binding association kinetics (Y. von Hansen, R.R. Netz and M. Hinczewski, J. Chem. Phys. 132, 135103 (2010).

In our talk, we will discuss the possibility to exploit versatile simulations at the mesoscopic level in order to take into account simultaneously the dynamics of the filament, the diffusive approach of the protein towards the active site, the binding reaction events and the solvent bath. Some preliminary results on this association kinetics using the MPCD technique will be presented. Such simulations should be particularly useful to explore living filament kinetics in various environments, such as close to a surface or a membrane, in concentration gradients, etc..).