Seminar

"IRTG: Soft Matter Science "

Polymers and Nanoparticles: Theory and Computer simulations

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Wednesday, February 9, 14h15

"Hörsaal Makromolekulare Chemie",
Stefan-Meier-Str. 31, Freiburg

You are welcome to meet Pr. Jens-Uwe Sommer after the seminar. Do not hesitate to contact Christelle Vergnat (softmattergraduate@physik.uni-freiburg.de) to organize a meeting.

Polymers and Nanoparticles: Theory and Computer simulations

We consider various problems of polymer-nanoparticle-interactions using theoretical methods and computer simulations. For nanoparticles immersed in a polymer solution depletion attraction is the major driving force for aggregation of nanoparticles under athermal conditions. Using Molecular Dynamics we show that the interactions between nanoparticles mediated by the polymeric environment do not depend on chain length if the polymer solution is above the overlap threshold. Using simple arguments we demonstrate that the attraction force in the athermal case is proportional to product of the osmotic pressure and the correlation length of the polymer solution. Such forces are strongest in the melt state. A particular interesting system for applications are nanoparticles in contact with polymer surfaces such as polymer brushes. Here, different regimes for the adsorption of nanoparticles can be found. For weak attraction between the polymer brush and the nanoparticles surface adsorption on top of the brush is found while for stronger interactions nanoparticles are absorbed inside the polymer layer. We outline simple scaling models to explain the behavior obtained in computer simulations. We propose some intriguing possibilities to combine nanoparticles and polymer brushes to achieve switchable surface. Finally, aspects of protein-adsorption in charged polymer brushes are discussed.