INSTITUTE FOR COMPUTATIONAL PHYSICS

Universität Stuttgart

Einladung zum ICP-Kolloquium (online)

via zoom https://zoom.us/j/97025760013?pwd=SjAzaGlNdlJTbndIdkpxUzBtdzIyQT09
Meeting ID: 970 2576 0013, Passcode: 716796

Auskunft: Dr. Alexander Schlaich, Tel: 0711 685 63607

Prof. Dr. Joachim Dzubiella
Physikalisches Institut, Universität Freiburg

hält am

Donnerstag, 20. Mai 2021, 16:00 Uhr

einen Vortrag über das Thema:

"On the permeability of dense polymer membranes for the selective transport of molecular solutes"

Abstract:
The permeability of polymers for the selective transport of molecular penetrants (drugs, toxins, reactants, etc.) is a central property in the design of soft functional materials. However, the permeation of dense and hydrated polymer membranes is a complex molecular-level phenomenon, and our understanding of the underlying physicochemical principles is still very limited. Here, I present our recent modeling efforts using coarse-grained as well as atomistic computer simulations in combination with the linear-response solution-diffusion model to understand and quantify the permeability of dense polymer (networks). Our work reveals some universal physical principles, such as strong solute partitioning-diffusion cancellation effects for a wide parameter regime, as well as significant 'chemical' effects (such as solute polarity and shape) which all contribute to the control of permeability. The gained insights enable us to formulate semi-empirical rules and scaling laws to potentially describe and extrapolate the permeability also for other polymer/solute systems.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Apl. Prof. Dr. R. Hilfer
Apl. Prof. Dr. M. Fyta