

GRK 2516 Soft Matter Seminar

April 28, 2022 at 3 p.m.
Minkowski Room, 05-119, Staudingerweg 7

Research seminar of the DFG Research Training Group GRK 2516 (<https://grk2516.uni-mainz.de>).

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Molecular Dynamic Simulation of Free chain Diffusion into a Regular Network

Thermo-sensitive hydrogels have attracted considerable attention in the field of bio chemistry and bio-medicine. Earlier works show that microfluidics can be used to create core-shell particle with decoupled elasticity and surface adhesiveness. However these experiments could not achieve proper control over the core-shell interconnectivity. We use MD simulations to understand and quantify the diffusive interpenetration of these shell polymers into a core gel. The simulation uses a Regular network to model the gel which is diffusively invaded via a polymer solution. We look into the interfacial profile and the ways to control this core-shell connectivity. The density profiles show a clear dependence of penetration on shell polymer concentrations. This is also seen in the degree of interfacial integration and diffusion depths. Finally the analysis of diffused free chain within the gel shows the emergence of large clusters leading to percolation. These results give us insight into how the factors like the core-shell polymer contact time, shell polymer concentration, etc can help us fine tune the core-shell connectivity in experiments.