Thomas Speck
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JOHANNES GUTENBERG UNIVERSITÄT MAINZ

GRK 2516 Soft Matter Seminar

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None

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

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Multiscale modelling of advanced materials and interfacial phenomena

Interfaces between different materials are ubiquitous in natural systems and in technological applications. Often, the interface gives rise to interesting phenomena that significantly affects the behaviour of the system. I will present studies of the interfacial behaviour in two types of system: a) polymer composites and b) heterogeneous nucleation.

Polymer composites are typically comprised of filler particles, such as carbon fibres, or inorganic nanoparticles, embedded in a polymer matrix. Filler particles are added to alter the polymer properties, for example, to create lightweight and high strength composites that are widely used in the aerospace and automotive industries. The interfaces between the polymer and filler particles, determine the overall properties of the composite material. Simulations can provide molecular level insight into the interfacial structure and properties, which is extremely challenging to measure experimentally. I will show how simulations have provided insight into the properties of polymers at a solid interface [1-3].

Crystal nucleation from solution is known to mainly occur at interfaces (heterogeneous nucleation), although the mechanisms are not well understood. Experiments on glycine aqueous solutions found that oil and PTFE interfaces dramatically accelerates glycine nucleation compared to an air–-solution interface [4,5]. Molecular dynamics simulations found significantly enhanced vs depleted glycine concentrations at the oil-solution vs air-solution interfaces, respectively, which explains the observed nucleation behaviour [5].

[1] K. Johnston and V. Harmandaris, Soft Matter 8, 6320 (2012)
[2] K. Johnston and V. Harmandaris, Macromolecules 46, 5741 (2013)

[3] D. McKechnie et al. Polymer 195, 122433 (2020)
[4] M. J. Vesga et al. Cryst. Eng. Comm. 21 2234 (2019)
[5] D. McKechnie et al. J. Phys. Chem. Lett. 11, 2263-2271 (2020)

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