

GRK 2516 Soft Matter Seminar

Sept. 14, 2023 at 2:30 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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Modeling drying-induced assembly in colloidal suspensions

Materials made from nanoparticles (NPs) have highly versatile applications, ranging from household products such as paint to functional materials used for catalysis and optoelectronics. The properties of such materials can be tailored through the chemistry of their NPs as well as the NP composition within the material. A common method to prepare such materials is to disperse the NPs in a solvent at a low volume fraction, then remove the solvent to assemble the NPs into a solid. For example, solvent drying from planar surfaces has been used to make abrasion- and bacteria-resistant NP coatings, while solvent drying from spherical droplets has been used to make porous supraparticles with significant internal void space that is promising for catalysis, photonics, and sorption. The mesoscopic structure of the NPs within these materials is known to depend on both properties of the NPs and the drying conditions; however, predicting it is challenging because the NP self-assembly involves confined molecular thermodynamics and nonequilibrium transport. In this seminar, I will discuss our efforts to use both particle-based simulations and continuum modeling (dynamic density functional theory) to model drying-induced assembly in colloidal suspensions. The two types of models shed different insights into the self-assembly process at different scales. Our principal finding is that solvent-mediated hydrodynamic interactions between NPs play a critical role in the drying process that must be captured to faithfully resolve the final structure in many cases. In future, we envision using these models to design NPs and drying processes to assemble them into materials with targeted compositions.