Evaporation-induced structure formation in colloidal suspensions

A talk by Michael P. Howard
Department of Chemical and Biological Engineering,
Princeton University, New Jersey, USA

DATE / TIME: Thursday, 22nd of March 2018, 04:00 p.m.

LOCATION: TU Vienna, Seminar Room 138C (Freihaus, Tower B/yellow, 9. OG)

A common method to prepare a solid coating or a crystal of colloidal particles is to first disperse the particles in a liquid solvent and then dry the suspension by evaporation. Evaporation increases the colloid concentration, ultimately leaving a close-packed solid after the solvent is removed. Despite the conceptual simplicity of this process, the influence of the evaporation conditions on the final solid structure is still not fully understood due to a slew of effects, including solvent-mediated hydrodynamic interactions between particles, which are challenging to model. In many situations, the structures that form after evaporation are amorphous or polycrystalline and difficult to predict. Recently, we have applied nonequilibrium molecular dynamics simulations to understand evaporation-induced structure formation for two processes:

crystallization and vertical segregation. First, we show how a colloidal crystal nucleates and grows from a drying air-solvent interface, and use a machine-learning approach to automatically discover and characterize interfacial and defective structures. Complementary implicit-solvent simulations demonstrate the nontrivial role that the solvent plays in controlling the crystallization process. We then show how nonequilibrium vertical segregation is induced by size in drying polydisperse colloidal mixtures using implicit-solvent simulations. We quantify how this segregation depends on both the mixture properties and the drying rate, and propose a model for it based on dynamical density functional theory. Our work has important implications for the processing of colloidal suspensions and more generally for nonequilibrium molecular modeling.