Kolloquium
Theoretische Physik
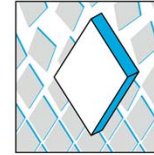
Universität
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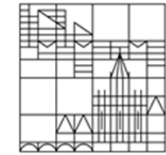
Prof. Dr. Baron Peters
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Two vignettes on nucleation: I. Acceleration by trace additives, and II. Modeling LaMer Burst nucleation

Part I. Trace additives exert control over nucleation and polymorph selection in many natural and industrial environments. We propose a theoretical model that predicts changes in nucleation barriers based on the adsorption properties and concentrations of trace additives. The model is based on classical nucleation theory and a statistical mechanical model for Langmuir adsorption. The model accounts for fluctuating additive coverage at the nucleus-solution interface. The model also incorporates diffusion controlled attachment/detachment models for the solutes and additives. Theoretical predictions closely follow the computational results from a Potts-lattice gas model that includes solvent, solute, and surfactant-like species. We will examine surfactant binding strength, concentration, and oligomerization as ways to modulate the potency and selectivity of additives for controlling nucleation.

Part II. Recent efforts to synthesize monodispersed nanoparticles have employed in situ reactions to steadily and homogeneously increase solute supersaturation. As the supersaturation climbs past a critical level in solution, the nucleation rate spikes giving birth to a large population of homogeneously formed nuclei over a very short interval of time. Subsequent growth of these nuclei lowers the supersaturation and thereby suppresses further nucleation. The result is a large population of nearly monodisperse particles. Classic experiments by T. Sugimoto and others have been modeled with deterministic models having separate stages of supersaturation build-up, nucleation, growth, and sometimes ripening. We examine assumptions in these models and extend them. We also reformulate the models to account for size dependent growth rates, supersaturation dependent nucleation rates, etc. Finally, we present a fully non-equilibrium stochastic model for LaMer burst nucleation. We discuss differences between these models and the kinetic parameters that emerge from using them to interpret nucleation/growth data (chalcogenide nanoparticle synthesis (Prof. J. S. Owen) and gold nanoparticle synthesis (Prof. S. L. Scott).