Solvay Seminars in Macromolecular Science & Engineering

Macromolecules Innovation Institute (MII)

VIRGINIA TECH

Prof. Athanassios Z. Panagiotopoulos

"Stratification and Crystallization in Drying Colloidal Suspensions"

Princeton University
Susan Dod Brown Professor
Department of Chemical and Biological Engineering

Host: Shengfeng Cheng

Abstract: Drying colloidal mixtures can undergo a spontaneous, nonequilibrium vertical separation (stratification) into layers enriched in particles of a specific size, an effect which can be exploited to create functional coatings. It was recently observed that for large particle size ratios and drying rates, smaller spherical colloids migrate to the top of the film, while big spherical colloids are pushed to the bottom, creating a peculiar and counterintuitive "inverted" stratification. To investigate this behavior, we performed simulations of binary mixtures of colloids and quantified the stratification dynamics in detail. Interestingly, inverted stratification was observed even at moderate drying rates, but the thickness of the stratified layer decreased. In addition, polymer-polymer and colloid-polymer mixtures were also studied. A model based on dynamical density functional theory was proposed to explain the observed phenomena. We have also investigated the influence of hydrodynamic interactions on stratification. Our simulations show, that it is critical to incorporate hydrodynamic interactions into models and simulations in order to reliably predict stratification in drying mixtures. In the second half of the talk, I plan to describe simulations of evaporation-induced crystallization, in which in drying colloidal suspensions and discuss the influence of drying rate on the quality of the crystals that form. In order to characterize the character of the drying suspensions, the group has developed autonomous crystal structure characterization methods using non-linear dimensionality reduction and machine-learning techniques.

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Bio: Prof. **Thanos Panagiotopoulos** received an undergraduate degree from the National Technical University of Athens and a PhD from MIT, both in Chemical Engineering. After a postdoctoral in Physical Chemistry at the University of Oxford, he has held faculty positions at Cornell and the University of Maryland; he is currently the Susan Dod Brown Professor and Department Chair of Chemical and Biological Engineering at Princeton University. He is a member of the U.S. National Academy of Engineering and the American Academy of Arts and Sciences. He is the author of more than 280 technical articles and of the undergraduate textbook "Essential Thermodynamics."

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