Weekly Seminar

Mesoscale Solubilization in Aqueous Solutions of Hydrotropes

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Time: 4:00pm, April. 17, 2013 (Wednesday)
时间：2013年4月17日 （周三）下午4:00
Venue: Room 607, Science Building 5
地点：理科五号楼607会议室

Abstract

Hydrotropes are amphiphilic molecules, too small to cause spontaneous self-assembly towards equilibrium mesoscale structures in aqueous solutions, but they form dynamic, noncovalent assemblies, which may create microscopic regions of lowered polarity. This enhances the solubilization of hydrophobic compounds in aqueous solutions and may cause further aggregation to larger structures In this work, unusual mesoscopic properties of aqueous solutions of a non-ionic hydrotrope, namely tertiary butyl alcohol (TBA) have been investigated by light scattering, small angle neutron scattering, and molecular dynamics simulations. Aqueous TBA solutions show anomalous thermodynamic and structural properties in the range of concentrations ~ 3–8 mol % TBA and temperatures ~ 0–25 °C . These thermodynamic anomalies appear to be associated with short-lived, short-ranged micelle-like structural fluctuations, distinctly different from usual concentration fluctuations in non-ideal solutions. Molecular dynamics simulations of aqueous TBA solutions show clustering of TBA molecules on a nanometer scale, interacting through hydrogen bonds with a shell of water molecules. In this concentration and temperature range, we have found that TBA aqueous solutions, on the addition of a third, more hydrophobic component, show the presence of mesoscopic inhomogeneities of size about a 100 nm. Experiments and simulations with controlled addition of a third component, such as cyclohexane, reveal the mechanism of formation of these inhomogeneities through stabilization of micelle-like fluctuations by the hydrophobic component These mesoscopic structures are long-lived, i.e., stable up to many months We have confirmed that stable aqueous colloids can be created with small molecules, without involvement of surfactants or polymers Such kind of novel materials may find applications in various process and product designs in pharmaceuticals, agrochemicals, cosmetics and food industry

About the Speaker

Mikhail A. Anisimov got his PH.D degree in Moscow State University, Russia in 1969. He is currently a professor in Department of Chemical & Biomolecular Engineering and Institute for Physical Science & Technology, University of Maryland, College Park He received many awards and recognitions He is a foreign member of the Russian Academy of Engineering, and a foreign member of the Russian Academy of Natural Sciences as well as a member of the New York Academy of Sciences He is in the Editorial Board of several journals His research interested includes the theoretical and experimental studies of mesoscopic fluctuations in soft matter, both in molecular fluids and in complex fluids. He published more than 200 publications in this fields.