Statistical thermodynamics of fluids with mesoscopic inhomogeneities

Atoms, molecules or colloidal particles are uniformly distributed in space if thermal motion at high temperature does not allow for condensation. If temperature is sufficiently low and molecules tend to stay at the minimum of the potential energy, then the homogeneous distribution becomes unstable for a certain range of density. In simple fluids, liquid and vapor phases coexist in such conditions. In the case of charged macromolecules or nanoparticles, the sum of all interactions in some solvents may lead to attraction at small distances and repulsion at large distances. If the repulsion is strong, then instead of the liquid-vapor coexistence, aggregates are formed. The size of the aggregates is determined by the range of attraction, while the distance between them is determined by the range of repulsion. In water solutions of lipids, which are composed of water soluble and water insoluble parts, micelles or bilayers are formed, where the insoluble part is hidden inside the aggregates.

In living organisms the key role is played both by lipids which form cell membranes, and by charged macromolecules which form aggregates. Amphiphilic molecules and charged particles are also components of soft matter. Self-assembly has numerous applications and enormous potential to be applied in future.

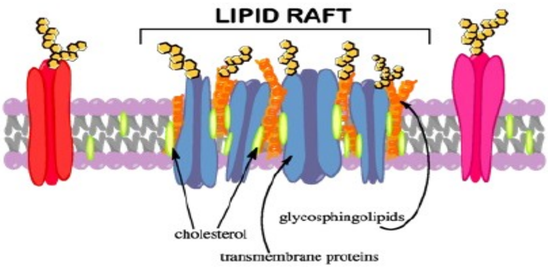

Fig. 1 Schematic representation of a lipid bilayer containing aggregated proteins.

In biological systems a cell and organelles are surrounded by an elastic membrane. A mismatch between the system size and the typical distance between the aggregates may lead to a change of the size and number of aggregates, and to numerous anomalies, such as increasing pressure with increasing volume. Inclusion of aggregating molecules in confined space was important for origin of life. In this project we will investigate the influence of walls of different shape, rigid or elastic, permeable or not, on spontaneous aggregation.

Liquid crystals of cubic symmetry, where the mid-plane of the lipid bilayer has a shape of a saddle in each point, are particularly intriguing. Such a bilayer separates two branched and disjoint water channels. An important example of the bicontinuous structure is the endoplasmic reticulum.

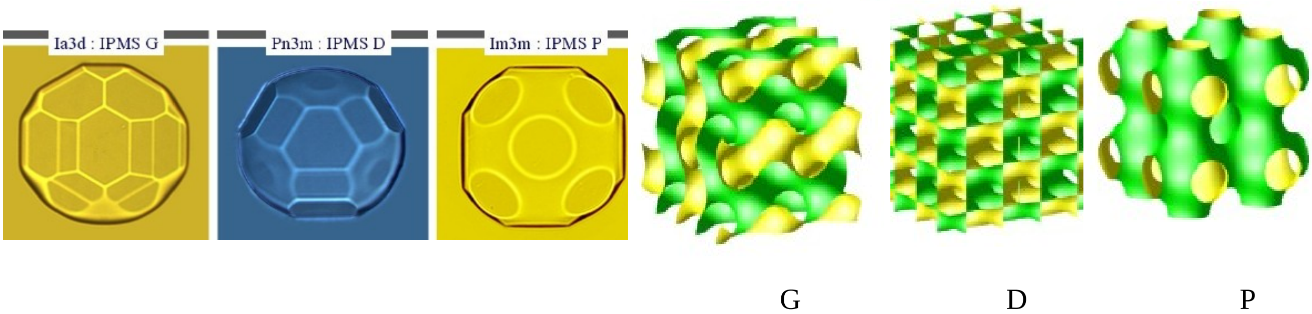

Fig.3 Monocrystals of Ia3d (G), Pn3m (D), Im3m (P) phases and their inner structure

Nanoparticles of these phases, cubosomes, can be used as carriers of drugs soluble either in water or in organic solvent. In this project we are going to investigate liquid crystals with nontrivial inner structure.

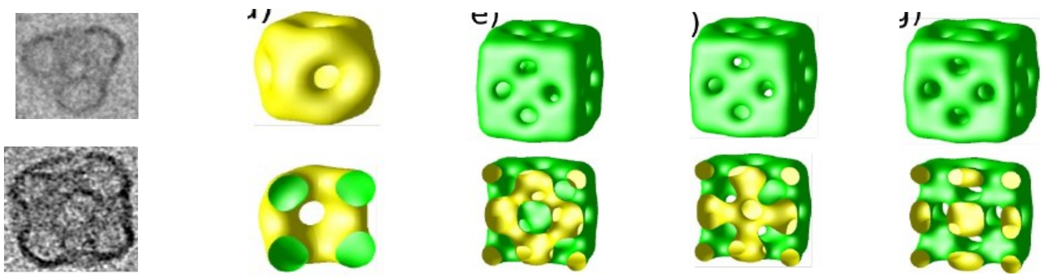

Fig. 4. Small cubosomes. The images from Transmission Electron Microscope [Angelov et al Langmuir **28**, 16647 (2012)] and theoretically obtained surfaces which show the location of the amphiphilic bilayer. In the upper row whole cubosomes are presented, and in the lower row their cross-section is shown.