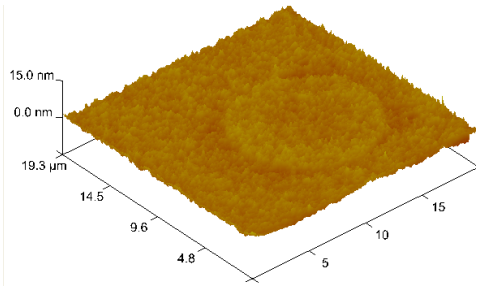
NIRT: Aerogels and Related Nanoporous Materials for Biological Membranes

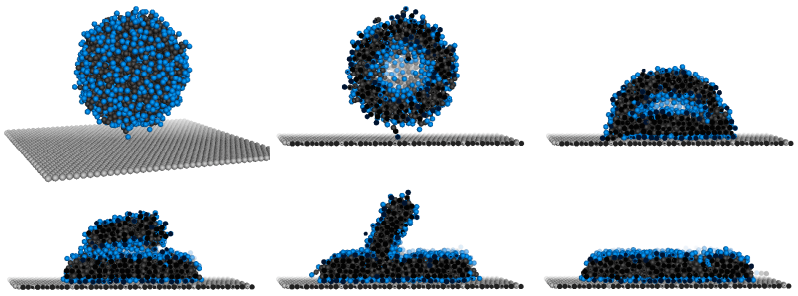
NSF NIRT Grant 0506602

PIs: **Subhash Risbud[1], Roland Faller[1], Margie Longo[1], Curt Frank[2]**
[1]UC Davis, [2]Stanford University



AFM image of phase-separated lipid bilayer on xerogel

In the first grant year we achieved the formation of xerogel supported lipid bilayers containing lateral heterogeneities. Vesicles of mixtures of two phase separating lipids were deposited onto a xerogel substrate. By AFM imaging a nanometer-scale undulation was observed to be superimposed upon the phase-separated bilayer indicating that the bilayer may be following closely the surface. This observation requires closer inspection of the accessibility of the proximal leaflet to the aqueous environment between the xerogel particles. We are installing two new techniques that will be ideal for this. Fluorescence interference contrast microscopy is a non-contact technique (unlike AFM) which gives nm height resolution and sub µm lateral resolution. It will be used to determine if the bilayer exists substantially (10s of nms) above the xerogel bead surface or if it is in intimate contact as our AFM images indicate. Single particle tracking gives trajectory information of single lipids with nm lateral resolution and should allow us to trace out the footprint of the beads on the proximal leaflet. Other techniques such as Cobalt Quenching will also give a percentage of the bilayer accessible to the aqueous space. The computational side of the project in the Faller group started with the implementation of confining surfaces in the existing computer models. Two students were trained using the *Gromacs* and *ESPResSo* (co-developed by collaborator Deserno) molecular modeling suites. We mainly focused on the use of ESPResSo as it is most useful for studies on the important length scales. We were able to model the interaction of simple surfaces with vesicles and bilayers. This leads naturally into the area of topographically patterned surfaces such as an aerogel or xerogel. We are developing an aerogel model on the same length scale as the experiments implementing mixed bilayers to study static and dynamic heterogeneities. These simulations will be enhanced in two directions. We strive for higher resolution and atomistic detail and we plan the implementation of simple proteins. An alternative nanoporous substrate is nanoporous alumina which may be formed by application of an anodic current to an aluminum substrate in 0.3M oxalic is studied in the Franck group and results in a close-packed hexagonal pore array. Pore sizes range from 10 nm up to 400 nm, and may be controlled by varying the anodisation conditions and post processing of the porous surface. Both bulk aluminum and thin films may be used for pore formation. Coupling of the nanoporous surface to other characterization tools, such as quartz crystal microbalance will allow detailed analysis of vesicle fusion and membrane formation.


ESPResSo modeling of supported bilayer formation