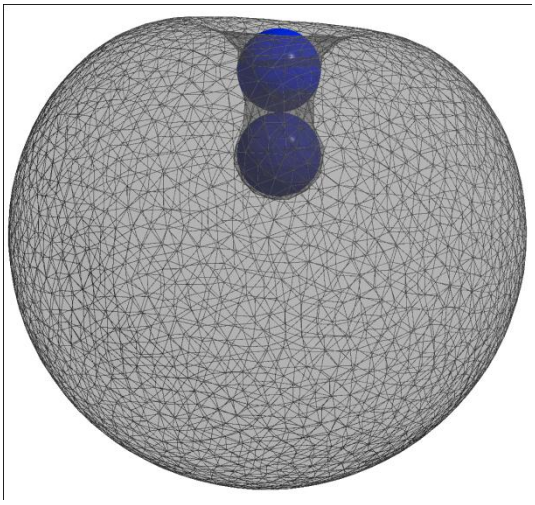
Project B1: Cooperative wrapping and membrane permeation of nanoparticles

Project leader: **Weikl (MPIKG)**
Co-supervisor: **Gradzielski (TUB)**
US partner: **Hall (NCSU)**

Outline. Recent advances in nanotechnology have led to an increasing interest in how nanoparticles interact with biological matter. Nanoparticles can permeate biomembranes by wrapping and subsequent fission of a membrane neck that connects the membrane envelope of the wrapped nanoparticles to the remaining membrane. The wrapping requires favorable adhesion energies between the nanoparticles and the membrane to compensate for the energetic cost of membrane bending. In the first funding period, theoretical approaches based on energy minimization have led to novel tubular membrane structures that wrap linear aggregates of spherical nanoparticles (see figure). The high stability of these particle-filled membrane tubules implies cooperative wrapping and strongly attractive membrane-mediated interactions between the particles. In this project, we will investigate how the shape and softness of the nanoparticles affects their membrane-mediated interactions and wrapping cooperativity. In addition, we will investigate the dynamics of the wrapping process.



Monte Carlo snapshot of two spherical particles wrapped by a lipid vesicle. In this example, the total energy, which is the sum of the bending energy of the vesicle and the adhesion energy of the particles, is minimal if the particles are wrapped cooperatively by a membrane tubule.

Research within the German group. The doctoral researcher working on this project will perform Monte Carlo simulations of nanoparticles in contact with a lipid vesicle. The focus will be on particles with non-spherical shapes, e.g. with oblate or prolate shapes, and on soft particles. A central question is how the stability of the recently found membrane tubules that wrap several particles depends on the shape and softness of the particles. The softness of the particles due to polymer shells will be taken into account by the interaction potential between the particles and the vesicle membrane. In Monte Carlo simulations, the membranes are modeled as triangulated surfaces. The interaction potential of the particles and the vesicle depends on the distance of the particles from the vertices of the discretized membrane.

Longer-term perspective. Later in the project we will investigate the wrapping and permeation dynamics with molecular dynamics simulations and Monte Carlo simulations. We will consider the dynamics of the fission step in molecular dynamics simulations with a coarse-grained model of lipid membranes.

Complementary work in US partner group. The molecular dynamics simulations will be carried out in cooperation with Hall, who has developed a coarse-grained molecular model of lipids suitable for fast discrete molecular dynamics simulations. We will consider the wrapping of small nanoparticles, which involves high membrane curvatures with radii close to the membrane thickness, and the fission step of nanoparticle permeation.

Status of the project. The project will be in close collaboration with project B2 (Gradzielski) in which the interactions of soft nanoparticles with vesicle membranes will be studied experimentally. Computer simulations will also be employed in projects B3 (Grafmüller) and B5 (Schoen). Biomembranes are investigated experimentally in project C3 (Dimova) and theoretically in project C4 (Lipowsky).