1. **Description**

The phase behaviors of DPPC in aqueous solutions are investigated by MD-SCF simulations.



These two systems correspond to the system A and the system B in the page 13 of “Antonio De Nicola, Ying Zhao, Toshihiro Kawakatsu , Danilo Roccatano, Giuseppe Milano, Validation of a hybrid MD-SCF coarse-grained model for DPPC in non-lamellar phases, Theor Chem Acc (2012) 131:1167”. System A will form a reverse micellar hexagonal phase and system B will form a lipid bilayer phase.



1. **Systems**
2. System A:

Box size (nm): x=y=z=12.964; No. of particles: 21216; No. of DPPC: 1664; No. of water; 1248.

1. System C:

Box size (nm): x=y=z= 12.376; No. of particles: 18600; No. of DPPC: 300; No. of water; 15000.

1. **Commands**
2. Run the simulation by:

python scfA.molg

python scfA.gala --gpu=0 >a.log&

1. The PBC conditions can be removed by:

galaTackle filename.xml

Select the function of 9 and enter; a new “filename. reimage.xml” will be generated.

1. You can see the configuration by OVITO with XML files.