Nanoscale physics

The dynamics of water clusters embedded in phospholipid reverse micelles.

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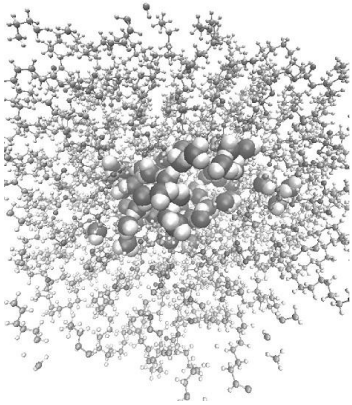
Molecular clusters confined in a variety of structures have been intensively studied for both scientific reasons and because of potential applications. Interesting case of molecular systems in nanoconfinement is the soft confinement - for example nanoclusters of polar liquids embedded in non-polar, hydrophobic environment.



Behavior of water in nano-scale soft confinement of phospholipid surfactant is interesting not only for our understanding of processes which take place inside living cells, but is also important from the point of view of applications. Soft confinement can also find potential applications as selective drug delivery carriers.

We performed a series of NVT molecular simulations (MD) of water molecules embedded in DMPC reverse micelle for temperatures ranging from 280 to 320 K. Spherical periodic boundary conditions were applied to the studied systems. The following observables were calculated and discussed: mean square displacement, water – water pair distribution function, total water dipole autocorrelation function, translational diffusion coefficients and activation energy.