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Coarse-Grained Molecular Simulation of Lipid Self-Assembly

WATARU SHINODA, National Institute of Advanced Industrial Science and Technology

The talk will review our recent work on understanding the behavior of lipid self-assembly using a coarse-grained (CG) force field model developed recently [1]. The CG model is designed to reproduce experimental surface/interfacial properties as well as distribution functions from all-atom (AA) molecular dynamics (MD) simulations. A series of MD simulations has elucidated that the CG model reproduces the phase diagram reasonably and produces the membranes with reasonable elastic moduli, surface and line tensions. With a help of technical development of free energy computation, we have evaluated the stability of liposome. [2] A comparison of CG-MD and a simple continuum theory for the free energy barrier to the vesicle-to-bicelle transformation reveals that the internal structural relaxation in the bilayer membrane plays an important role in lowering the free energy barrier in case of a small unilamellar vesicle. [2] The effects of lipid components and additives are also discussed in this talk. Especially the effect of fullerenes on the membrane properties will be discussed in details.[3] The behavior of fullerenes in the bilayer membrane and the resultant membrane properties depend on the size of fullerene and bilayer thickness quite sensitively. To discuss these details, we need a chemically accurate CG model constructed based on extensive AA-MD results.

[1] W. Shinoda, R. DeVane, M. L. Klein, Mol Simul 33, 27 (2007); ibid, Soft Matter 4, 2454 (2008); ibid, J. Phys. Chem. B 114, 6836 (2010); ibid, Soft Matter, 7, 6178 (2011).

[2] W. Shinoda, T. Nakamura, S. O. Nielsen, Soft Matter, 7, 9012(2011).; T. Nakamura, W. Shinoda, T. Ikeshoji, J. Chem. Phys. 135, 094106 (2011).

[3] R. DeVane et al. J. Phys. Chem. B, 114, 6386 (2010); C. Chiu et al. J. Phys. Chem. B 114, 6394 (2010). R. DeVane et al. J. Phys. Chem. B, 114, 16364 (2010); A. Jusufi et al. Soft Matter 7, 1139 (2011); C. Chiu et al. Soft Matter, 8 9610(2012).