Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Amphiphilic lipids in solution: a simulational study of lipid bilayer formation[1] THOMAS VOGEL, DAVID P. LANDAU, The University of Georgia, LILI GAI, KATIE A. MAERZKE, CHRISTOPHER R. IACOVELLA, CLARE M. MCCABE, Vanderbilt University, PETER T. CUMMINGS, Vanderbilt University and Oak Ridge National Laboratory — Amphiphilic molecules consisting of hydrophilic head and hydrophobic tail groups self-assemble into a wide variety of structures, such as bilayers (membranes), micelles, or vesicles (liposomes) when mixed with a suitable solvent. The understanding of this lipid self-assembly is essential for industrial, biological, or medical applications, but computer simulations are generally challenging due to the complex structure of the energy landscape. We show results for the lipid bilayer formation process obtained by newly developed parallel Wang–Landau Monte Carlo and statistical temperature molecular dynamics simulations. By applying those methods to a generic coarse-grained model for amphiphilic molecules in solution, we were able to obtain the thermodynamical data over the whole relevant temperature and energy range and to unravel the membrane formation process including all structural sub-transitions between different fluid and gel-phase bilayers.

[1]Research supported by NSF

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Date submitted: 09 Nov 2012 Electronic form version 1.4