Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Self-assembling structures resulting from the presence of polyelectrolytes in a solution of phospholipids[1] ROSS PACKARD, YVES DUBIEF, University of Vermont — The objective of this study is the characterization of self-assembled structures formed by the combination of phospholipids and polyelectrolytes. Coarse-grained molecular dynamics is used to simulate solutions of DPPC (1,2-Dipalmitoylphosphatidylcholine) and polyelectrolyes in three dimensional periodic domain. The MARTINI database defines the topology of coarse-grained macromolecules and water and simulations are performed using GROMACS. The interaction between negatively charged polyelectrolytes and positively charged hydrophilic heads of DPPC causes the disruption of lipid bilayer membranes and vesicles. The study attempts to define the conditions necessary for the formation of vesicles or organized networks of lipid bilayers that encapsulate the polyelectrolytes. Such structures are suspected to play an important role in biological fluids subject to large mechanical stress.

[1]The computational support of the Vermont Advanced Computing Center is gratefully acknowledged

Yves Dubief
University of Vermont

Date submitted: 21 Nov 2008 Electronic form version 1.4