Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effects of water models and simulation system size on dynamic heterogeneity of single component lipid membranes YOUNGHOON OH, JEONGMIN KIM, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — Biological membranes are composed of various different types of molecules and their composition is usually spatially heterogeneous. Recently it has been reported that the dynamics of lipids could also become spatially heterogeneous, where fast and slow regions of lipids could coexist. A recent simulation study showed that the diffusion of lipids even in single component lipid membranes could be spatially heterogeneous in liquid-ordered phase at sufficiently low temperature. [1] On the other hand, in the liquid-disordered phase at relatively high temperature, the dynamics of lipids was homogeneous in membranes. In this work, we systematically investigate the diffusion of lipids in single component DPPC lipid bilayers by employing three different water models (Big Multipole Water, Polarizable MARTINI and LJ MARTINI) and three different simulation cell sizes (L = 5nm, 10nm and 20nm). We find that even though the liquid-disordered to liquid-ordered phase transition occurs at different temperatures for different water models, the diffusion of lipids become spatially heterogeneous in liquid-ordered phases for all three different force fields. Reference [1] F. W. Starr, B. Hartmann, J. F. Douglas, Soft Matter, 10, 3036 (2014)

Younghoon Oh
Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea

Date submitted: 14 Nov 2014 Electronic form version 1.4