Abstract Submitted for the MAR10 Meeting of The American Physical Society

Field-theoretic model of membrane/protein assemblies KANG CHEN, GLENN FREDRICKSON, University of California Santa Barbara, KIM RASMUSSEN, PAUL WELCH, Los Alamos National Laboratory — We developed a coarse-grained field-theoretic model of an assembling membrane/protein system that includes immovable cylindrical transmembrane protein(s) and assembling membrane species including neutral and charged lipids, counterions, and water. This field-theoretic model is able to capture the molecular architecture of lipids that constitute the membrane. Our study focused on the following aspects: i) membrane thickness fluctuation due to hydrophobic mismatch, ii) the corresponding lipid tail stretching near the protein, iii) ion and cationic lipid distributions at various levels of protein head charge, iv) protein tilting, v) membrane-mediated protein-protein interactions, and vi) in-plane packing structures of proteins. Our simulations were used to evaluate free energies and structure that enabled the quantitative analysis of features such as lipid tail stretching and membrane/protein structural stability.

Kang Chen University of California Santa Barbara

Date submitted: 20 Nov 2009

Electronic form version 1.4