Abstract Submitted
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NaCl and Cationic lipid bilayer dynamics MARKUS S. MIETTINEN, Department of Applied Physics, Helsinki University of Technology, Finland, ANDREY A. GURTOVENKO, Institute of Pharmaceutical Innovation, University of Bradford, UK, ILPO VATTULAINEN, Department of Physics, Tampere University of Technology, Finland, MIKKO KARTTUNEN, Department of Applied Mathematics, University of Western Ontario, Canada — Positively charged lipid bilayer systems hold promise for safer and more efficient gene and drug delivery. Here we studied cationic bilayers comprising binary mixtures of cationic dimyristoyltrimethylammoniumpropane (DMTAP) and zwitterionic dimyristoylphosphatidylcholine (DMPC) lipids. Using molecular dynamics simulations we addressed the effects of bilayer composition (cationic to zwitterionic lipid fraction) and NaCl electrolyte concentration on the dynamical properties of these systems. We found that despite the DMPC lipids form complexes via Na^+ ions that bind to the lipid carbonyl oxygens, NaCl concentration had a rather minute effect on the lipid diffusion. The residence times of sodium ions in the carbonyl region appeared to lack a characteristic time scale, although observed a simulation period of over 200 ns. These prolonged dynamics of the sodium ions could be interesting for the physics of the whole membrane, especially to its interaction dynamics with charged macromolecular surfaces. 1. A. A. Gurtovenko *et al.*, J. Phys. Chem. B **109**, 21126 (2005) 2. M. Miettinen *et al.*, J. Phys. Chem. B,*(submitted)*

Markus S. Miettinen
TKK – Helsinki University of Technology

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