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**Lipid domains in zwitterionic-anionic lipid mixtures induced by combined effect of monovalent and divalent ions** HONGCHENG XU, Biophysics Program, University of Maryland, College Park, SAI GANESAN, Fischell Department of Engineering, University of Maryland, College Park, SILVINA MATYSIAK, Biophysics Program, Fischell Department of Engineering, University of Maryland, College Park — Lipid domain formation is an important process for many cellular processes. In experiment, the effects of $Ba^{2+}$, $Sr^{2+}$, $Ca^{2+}$ and $Mg^{2+}$ in inducing lateral phase separation in the binary phosphatidylcholine-phosphatidylserine (PC-PS) bilayer are quite different, of which the molecular mechanism remains to be understood. We have explored the effect of monovalent (MI) and divalent (MII) cationic radii on lipid domain formation in mixed zwitterionic-anionic lipid bilayers. We propose a mechanism for the formation of divalent-cation-induced lipid domains based on MD simulations with our Water-Explicit Polarizable MEMbrane (WEPMEM) coarse-grained model, which uses PC as the model for zwitterionic and PS for anionic lipids. Lipid aggregation only occurs with limited range of monovalent and divalent ion sizes in agreement with experimental observations. More ordering and closer packing of the lipids are noted within the domains, which correlate with bilayer thickness, curvature and lipid asymmetry. The results of the simulations reveal that the lipid domain consists of MII-mediated anionic lipid dimer/trimer complexes bridged by monovalent ions MI and provide a stereochemical insight in understanding the experimentally observed calcium-induced phase separation.

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