Electrodiffusion of Lipids on Membrane Surfaces

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Lateral random translocation of lipids and proteins is a universal process on membrane surfaces. Local aggregation or organization of lipids and proteins can be induced when this lateral random diffusion is mediated by the electrostatic interactions and membrane curvature. Though the lateral diffusion rates of lipids on membrane of various compositions are measured and the electrostatic free energies of predetermined protein-membrane-lipid systems can be computed, the process of the aggregation and the evolution to the electrostatically favorable states remain undetermined. Here we propose an electrodiffusion model, based on the variational principle of free energy functional, for the self-consistent lateral drift-diffusion of multiple species of charged lipids on membrane surfaces. Finite sizes of lipids are modeled to enforce the geometrical constraint of the lipid concentration on membrane surfaces. A surface finite element method is developed to appropriate the Laplace-Beltremi operators in the partial differential equations (PDEs) of the model. Our model properly describes the saturation of lipids on membrane surface, and correctly predicts that the MARCKS peptide can consistently sequester three multivalent phosphatidylinositol 4,5-bisphosphate (PIP2) lipids through its basic amino acid residues, regardless of a wide range of the percentage of monovalent phosphatidylserine (PS) in the membrane.