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Effect of Valence of Counterions on the Structure of Charged Membranes, a Computer Simulation Study BAOFU QIAO, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University — Phospholipids have been investigated for a long period, due to its ability of self-assembling into bilayer structures which resemble biological membranes. But most of the studies have been limited on the neutral phosphatidylcholine based lipids. The understanding of charged membranes (e.g., phosphatidylserine) is very limited due to the repulsion between the charged groups on lipids. In the present work, we investigated the effect of different counter-ions on the structures of charged membranes formed by 1,2-dilauroyl-sn-glycoro-3-phospho-L-serine. Three kinds of counterions were investigated, from monovalent, to divalent, to trivalent ions. Molecular dynamics simulations were performed at all-atom level. We have calculated the area per lipid. And the interaction between counterions and COO^- groups was found to dominate over that between counterions and PO_4^- groups.

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