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Molecular design and MD simulations of epitaxial superlattice of self-assembling ternary lipid bilayers GEORGE CHOU, MARK VAUGHN, K. CHENG, Texas Tech University — Multicomponent lipid bilayers represent an important model system for studying cell membranes. At present, an ordered multicomponent phospholipid/cholesterol bilayer system involving charged lipid is still not available. Using a lipid superlattice (SL) model, a 13 x 15 x 15 nm^3 ternary phosphatidylcholine/phosphatidylserine/cholesterol bilayer system in water with simultaneous headgroup SL and acyl chain SL at different depths, or epitaxial SL, of the bilayer has been designed with atomistic detail. The arrangements of this epitaxial SL system were optimized by only two molecular parameters, lattice space and rotational angle of the lipids. Using atomistic MD simulations, we demonstrated the stability of the ordered structures for more than 100 ns. A positional restrained system was also used as a control. This system will provide new insights into understanding the nanodomain structures of cell membranes at the molecular level.

George Chou
Texas Tech University

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