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Multiscale modeling of phospholipid bilayers: from explicit-solvent all-atom to solvent-free coarse-grained simulations ZUN-JING WANG, MARKUS DESERNO, Carnegie Mellon University — To advance the efficiency of phospholipid bilayer simulations and permit the treatment of challenging phenomena on mesoscopic length- and time-scales, several solvent-free Coarse-Grained (CG) phospholipid bilayer models have been presented in the past ten years. Most of them were derived in a top-down scheme, aiming to qualitatively reproduce phase diagrams, bending and stretching rigidity, area per lipid, and the thickness of a generic bilayer in experiments. Here, we derive a bottom-up CG model of an implicit-solvent lipid bilayer by matching its structural and mechanical properties with that of a membrane in all-atom resolution. Besides preserving chemical specificity and quantitative accuracy, we expect to gain a more fundamental understanding of the relationship between the elastic, mechanical, and diffusive properties of implicit solvent bilayers and their underlying CG interaction potentials, specifically bonded and non-bonded forces, as well as the effective interactions replacing the solvent.

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