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An Integral Equation Method Coupling with Variational Approach for Studying Coarse-Grained Lipid Dynamics SZU-PEI FU, SHIDONG JIANG, New Jersey Inst of Tech, ANDREAS KLÖCKNER, University of Illinois at Urbana-Champaign, ROLF RYHAM, Fordham University, MATT WALA, University of Illinois at Urbana-Champaign, YUAN-NAN YOUNG, New Jersey Inst of Tech — In macroscopic model, the well-known Helfrich membrane model has been extensively utilized as it captures some macroscopic physical properties of a lipid bilayer membrane. However, some phenomena such as membrane fusion and micelle formation cannot be described in this macroscopic framework. Yet the immense molecular details of a lipid bilayer membrane are impossible to be included in a plausible physical model. Therefore, in order to include the salient molecular details, we study the dynamics of coarse-grained lipid bilayer membrane using Janus particle configurations to represent collections of lipids These coarse-grained lipid molecules interact with each other through an action field that describes their hydrophobic tail-tail interactions. For this action potential, we adopt the integral equation method on solving energy minimizer with specific boundary condition on each Janus particle. Both the QBX (quadrature by expansion) and fhe fast multipole method (FMM) are used to efficiently solve the integral equation. We also examine the numerical accuracy and qualitative observation from large system simulations.

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