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A Theoretical Study on the Morphological Phase Diagram of Supported Lipid Bilayers. XIAN KONG, DIANNAN LU, ZHENG LIU, Tsinghua University, JIANZHONG WU, UC Riverside — Supported lipid bilayers (SLBs) are widely used in drug delivery, biosensors and biomimetic membranes. The microscopic mechanism of SLB formation and stability is complicated, depending on various factors underlying solvent-mediated lipid-lipid and lipid-substrate interactions. Whereas recent years have witnessed remarkable progress in SLB formation, relatively little is known about how to control SLB stability under diverse solution conditions for broader SLB usage and rational design. In this work, we examine SLB stability using a coarse-grained model in combination with the classical density functional theory (DFT) that accounts for ion-explicit electrostatic interactions, surface hydrophobicity, as well as the molecular characteristics of lipid tails. A morphological phase diagram is constructed for model SBLs in terms of various intrinsic properties of lipid molecules (such as lipid tail length, lipid head size and charge of polar head), substrate conditions (such as surface charge density and hydrophobicity), and solution parameters (such as ion concentration, ion type). The morphological phase diagram provides useful insights on the design and screening of SLB membrane for customized applications.

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