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Theory for registered and antiregistered phase separation of amphiphilic bilayers¹ JOHN WILLIAMSON, PETER OLMSTED, Georgetown University — Phase separation in bilayers can be exploited by nature, and engineers, to design-in function via membrane domains. The presence of two separate, yet coupled, leaflets forces one to ask whether and how such domains are aligned (registered) across the bilayer. Experiment and simulation yield intriguingly disparate observations. We introduce a theory for phase separation in coupled leaflets, by explicitly coarse-graining a lattice model that includes molecule-level structure and interactions. We show that hydrophobic mismatch leads to a complex competition of inter-leaflet couplings. The theory helps unify prima facie contradictory observations, by showing that domain antiregistration typically occurs as a metastable state, but can be kinetically preferred. The role of kinetics in governing registration/antiregistration is explored, the theory's predictions confirmed and illustrated with simulations, which show how a bilayer in the "spinodal region" can require nucleation to equilibrate. Our results shed light on a novel statistical mechanical problem of great practical importance, and motivate future work on intra- and inter-leaflet behaviour of bilayers. Reference: JJW and PDO, arXiv:1408.2744.

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