Abstract Submitted
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Physics of Polymersomes: lateral segregation experiments and raft simulations DENNIS DISCHER, Univ. Pennsylvania — Coupling between the inner and outer leaflets of a bilayer plays an important role in biomembrane function, particularly in inducing and registering rafts across leaflets for various cellular signals. However, mechanisms of raft registration remain elusive and several alternatives have been proposed, ranging from electrostatic coupling to chain interdigitation. A general mechanism has been suggested by recent experiments on Polymersomes in which binary mixtures of diblock copolymer amphiphiles exhibit domain registration upon ligand-induced segregation. Using coarse grained molecular dynamics (CGMD) simulations rooted in atomistics, raft registration arises spontaneously in bilayers with a calcium- or ligand-crosslinked ordered phase segregating from a liquid disordered phase. When rafts are not registered, a thickness mismatch between phases induces a "bump" in the apposing liquid phase leaflet, and the associated localized curvature guides rafts together stabilizing the registered state. The absence of explicit charge in the model and the fact that domain size modulates transmembrane coupling demonstrate that collective interactions are sufficient for raft registration. References: (1) D.A. Christian, et al. Spotted vesicles, striped micelles, and Janus assemblies induced by ligand binding. Nature Materials 8: 843–849 (2009). (2) D. Pantano, P.B. Moore, M.L. Klein, D.E. Discher. Raft registration across bilayers in a molecularly detailed model. Soft Matter 7, 8182-8191 (2011).

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