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Calculating energy barriers and activation states for steps of fusion

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Fusion between biological membranes is a widespread cellular process, responsible for events as varied as secretion of neurotransmitters and fertilization of egg by sperm. Molecularly, fusion is the merger of two lipid bilayer membranes, and this merger proceeds through several key intermediates states. But the transition energy barriers that separate these intermediates have not been determined. Using the string method, we calculate a least energy pathway and the activation states between intermediates for the entire fusion process. The bilayer energetics are based on a modified Helfrich Hamiltonian that accounts for long range interactions between bilayers, and a novel field theoretic treatment of hydrophobic potentials. Through the energetic analysis, we conclude that lipid demixing is required for the transition from a stalk to a hemifusion diaphragm, and that complete fusion is possible provided pore formation is initiated while the diaphragm is small. The calculations provide a movie of individual lipid deformations, as the membrane geometry and topology evolve over time.

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