Supporting Information:

Nanodroplets at Membranes Create Tight-Lipped Membrane Necks *via* Negative Line Tension

Vahid Satarifard, Andrea Grafmüller, and Reinhard Lipowsky*

Theory & Biosystems, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

July 26, 2018

Movie Captions

Movie1. Time-dependent engulfment of nanodroplet (dark blue) by lipid bilayer (green chains, yellow heads), viewed from the bottom and via two orthogonal cross-sections: The membrane tension is controlled by the lateral size $L_{\|}$ of the simulation box which is reduced, for fixed number of lipid molecules, from $L_{\|} = 130\,d$ at $t = 0$ to $L_{\|} = 120\,d$ at $t = 4\,\mu$s, with the basic length scale provided by the bead diameter d which is of the order of 1 nm. At $t = 0$, the droplet adheres to the bilayer membrane and is partially engulfed by it. As we reduce the box size $L_{\|}$ and thus the membrane tension with constant velocity $\mathrm{d}L_{\|}/\mathrm{d}t$, the contact area of the droplet with the membrane increases while the area of the $\alpha\beta$ interface decreases, see also Figure S1. The rotational symmetry of the membrane-droplet morphology is spontaneously broken at $L_{\|} = L_{\|}^{*} \simeq 124\,d$. For $L_{\|} < L_{\|}^{*}$, the morphology is characterized by a noncircular contact line and an elongated membrane neck. This non-axisymmetric morphology persists until the membrane neck closes, thereby attaining a tight-lipped shape. In Figure 2 of the main text, we display four snapshots of this movie.

Movie2. Shape and energy fluctuations of the nanodroplet (dark blue) partially engulfed by the bilayer membrane (green chains, yellow head groups) close to the morphological transition: (Top row) For fixed box size $L_{\|} = 125\,d > L_{\|}^{*}$, the membrane-droplet morphology is, on average, axisymmetric; and (Bottom row) For box size $L_{\|} = 122.5\,d < L_{\|}^{*}$, the morphology is non-axisymmetric. Note the different ordering of the individual free energy contributions: For $L_{\|} = 125\,d$, the largest contribution arises from the free energy of the $\alpha\beta$ interface (red) while the smallest contribution is associated with the bending energy of the bilayer membrane (green). For $L_{\|} = 122.5\,d$, on the other hand, the free energy of the $\alpha\beta$ interface represents the smallest contribution whereas the free energy of the contact line (blue) now makes the largest contribution.