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Supporting Material

New insights into BAR domain induced membrane remodeling

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Supplemental Material:

New insights into BAR domain induced membrane remodeling

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EM2 System setup and geometry

Figure S1 shows the initial conditions for the 250 nm diameter liposome EM2/SPAM simulations. The upper panel shows the relative length scales of a single N-BAR domain relative to the starting configuration for the liposome; the small yellow square on the liposome surface gives the rough size of a single N-BAR. The bottom panel shows the initial configuration of the EM2 liposome in the SPAM mesoscopic solvent. Initially, both the N-BAR density and membrane compositions, $\phi_{B,i}$ and $\phi_{M,i}$, were assigned random values ranging from -1 to 1. The 250 nm liposome employs 4000 EM2 quasiparticles while the 500 nm liposome contains 15436.

Figure S2 sketches two interacting EM2 quasiparticles. The entire EM2 membrane consists of a single sheet of pair wise interacting EM2 quasi-particles each separated by $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$ as given in Fig. S2 (a). For each quasi-particle, two additional unit vectors, designate the membrane normal vector, $\mathbf{\Omega}_\alpha$ and the orthogonal in-plane vector \mathbf{n}_α^T , $\alpha = i, j$. The resulting small angle between the two normal vectors is $\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j = \cos(\delta\theta_{ij})$. The curvature between the two EM2 quasiparticles, c_{ij} , is found from the membrane normal vectors as shown in Fig. S2 (a), $\delta\theta_{ij} / r_{ij} = 1 / R_{ij} = c_{ij}$, is the local curvature between the pair. Fig S2 (b) depicts the geometry the EM2 model adopts in a tube configuration.

Supplemental Tables

Table S1: Parameter ranges of the different terms in the mesoscopic model, Eq. 1, in the main manuscript

Term	Parameter	Tested values
H_S	a_B	0.001 amu (nm/ps) ²
H_{EM2}	k_c	10 k _B T
H_M	a_M	0.001 amu (nm/ps) ²
$H_{S,M}$	Λ_M^H, Λ_k^H	0.05 to 0.1 k _B T, 2.5 to 5 amu nm ⁴ ps ⁻²
H_O	Λ_O	5-15 amu (nm/ps) ²

Supplemental Figures

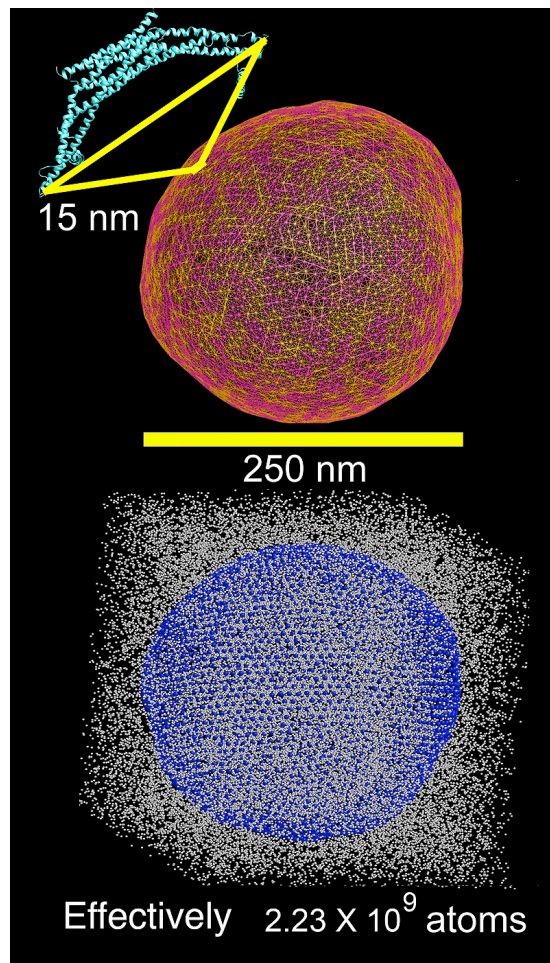


Figure S1: Snapshots of the EM2 liposome with surrounding mesoscopic solvent.

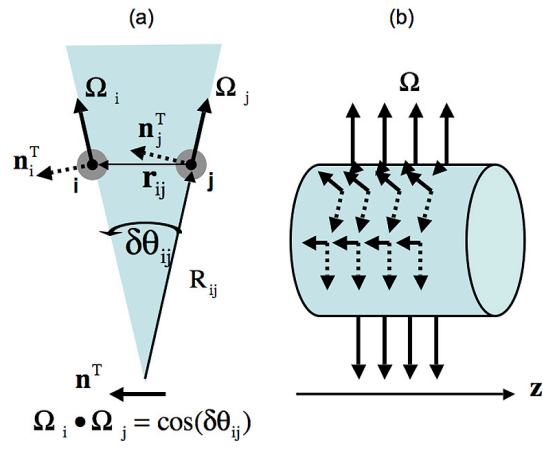


Figure S2: Panel (a) a schematic of the EM2 membrane quasi-particle geometry. Panel (b) the stabilization of tubules with the discrete EM2 membrane model.