Electronic Supplementary Material (ESI) for Soft Matter.

Supporting information for: Simulation of Fluid/Gel Phase Equilibrium in Lipid Vesicles

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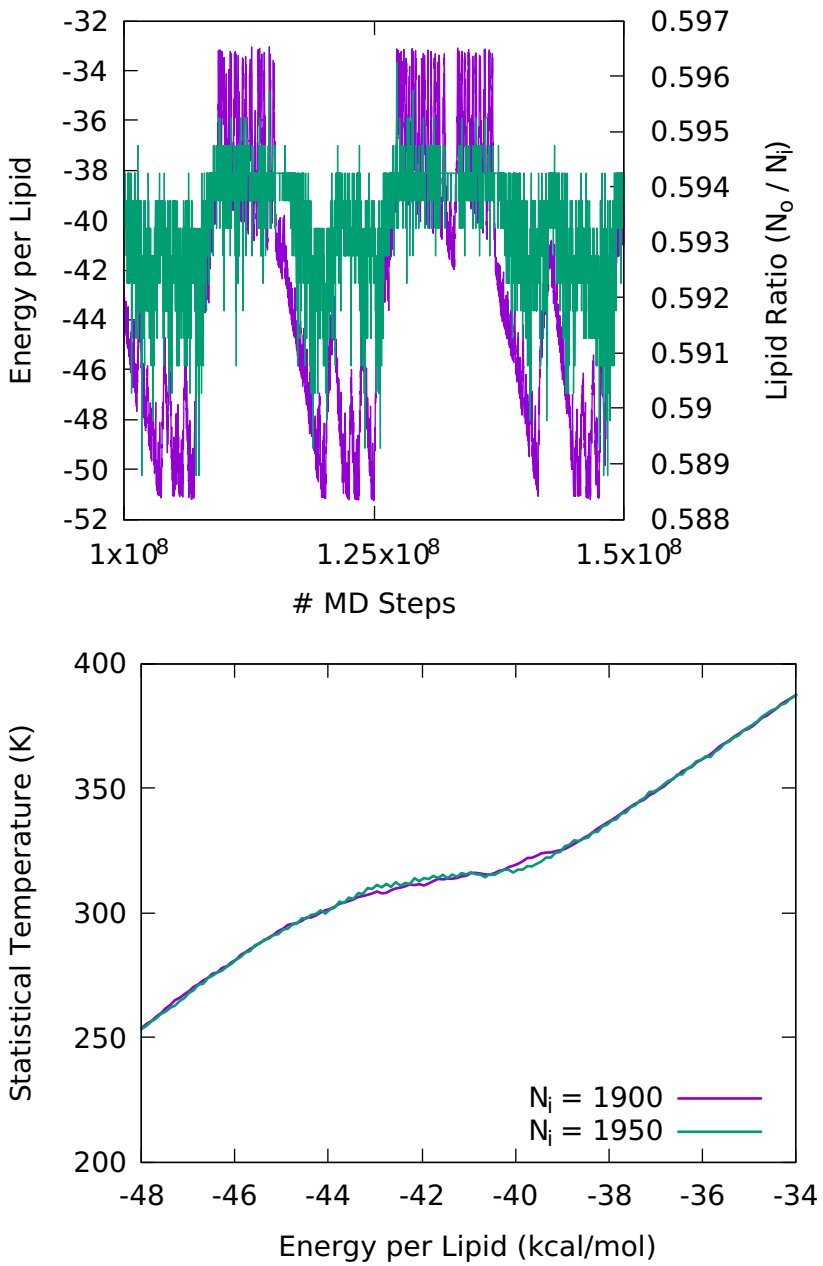

Figure S1: Top: Energy trajectory showing two transition events (purple) and trajectory of the outer / inner layer lipid ratio (green) showing that STMD finds lipid flip-flop events coupled to the transition. Bottom: $T_S(U)$ for different inner leaflet number $N_i/N_o = 0.59$ with $N_i = 1900$ (purple) and $N_i/N_o = 0.62$ with $N_i = 1950$ (green), with constant total $N = 5100$, as in the 20 nm vesicle. The transition is not particularly sensitive to minor changes to the initial lipid ratio, with only minor differences are present in the transition region. However, it is worth noting that large changes can prevent initial formation of a stable vesicle to begin with.

Movies of the trajectories showing a typical fluid→gel→fluid transition from the STMD trajectory are hosted on the Boston University Google Drive.

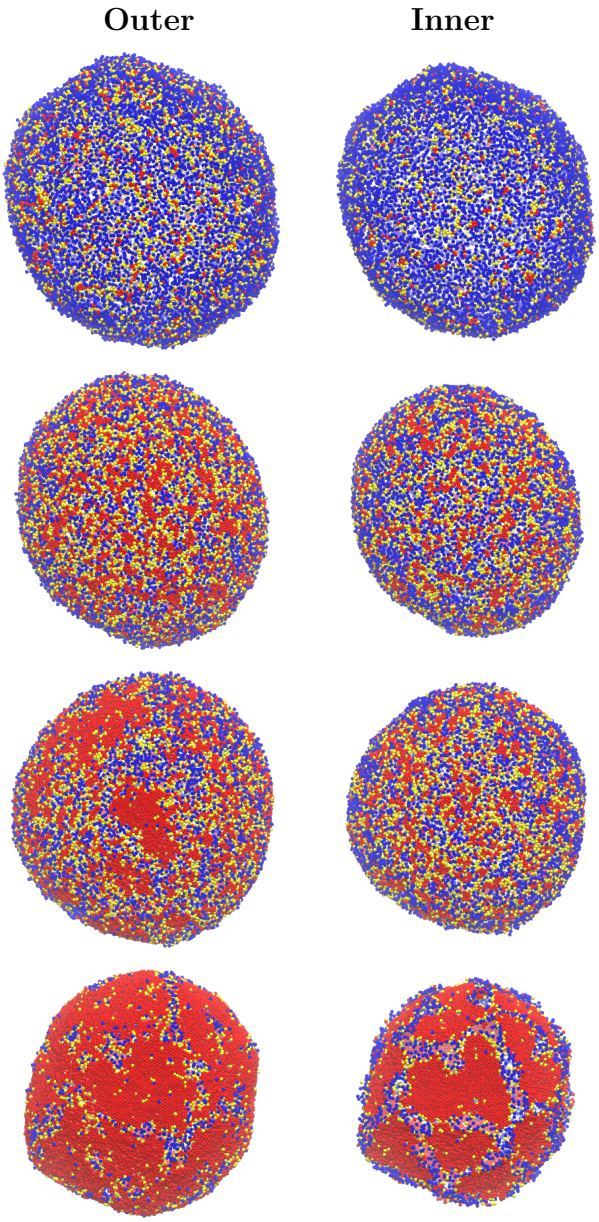

Figure S2: Snapshots of the 40 nm vesicle, with outer layer (left) and inner layer (right) during a typical freezing event. The same progression is followed as in the 20 nm vesicle and described in-text.

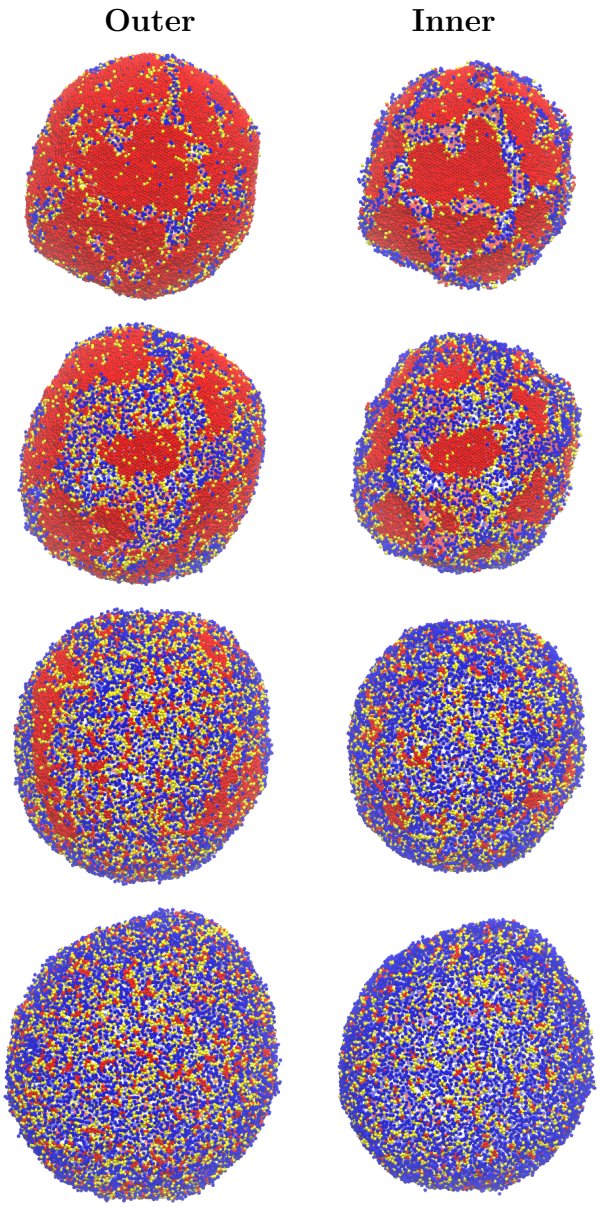

Figure S3: Melting of the 40 nm vesicle, with outer layer (left) and inner layer (right).

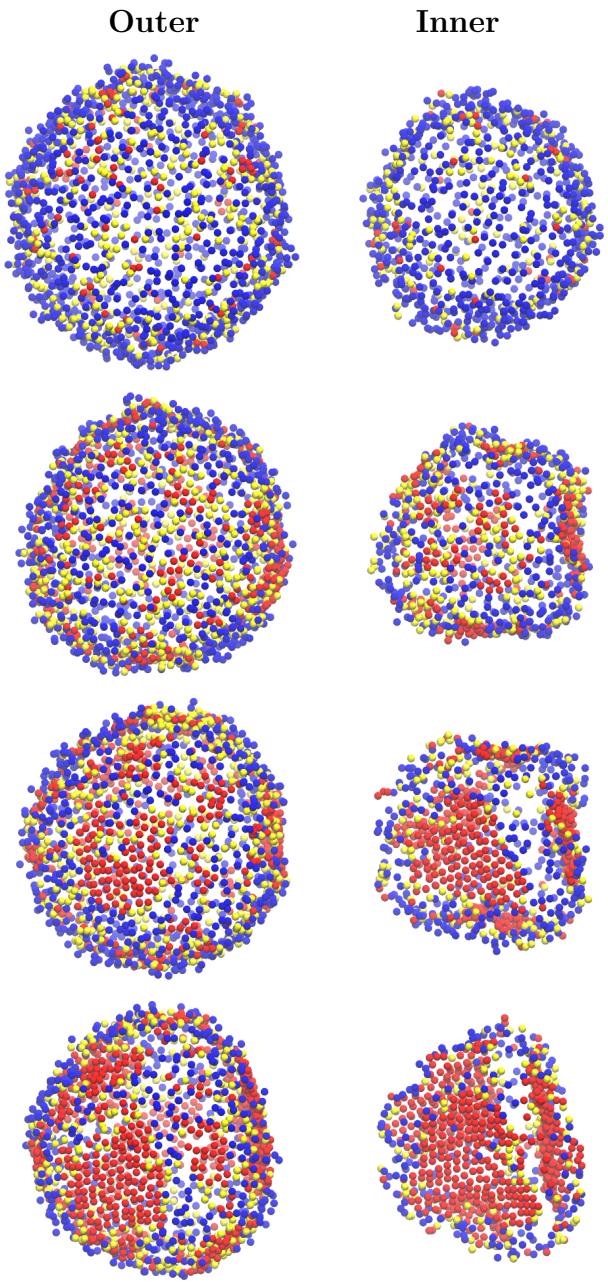

Figure S4: Freezing of the 10 nm vesicle. Outer leaflet is shown on the left and inner leaflet on the right. The most gel configurations are the least spherical due to large flat gel patches that form.

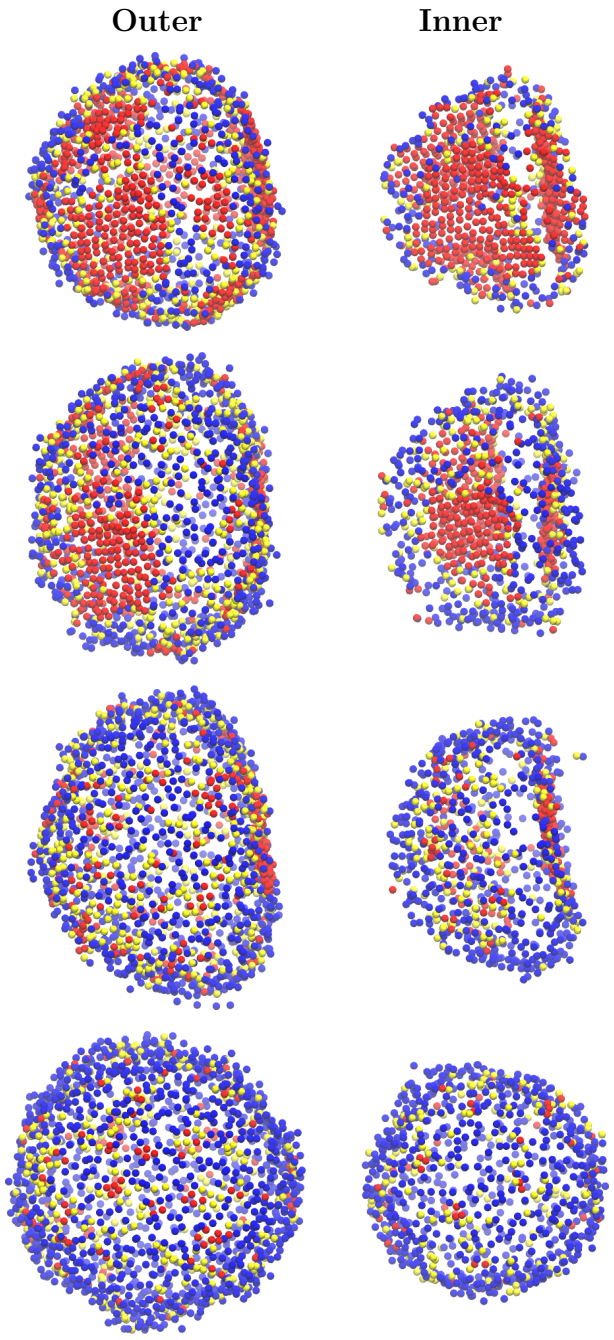

Figure S5: Melting of the 10 nm vesicle, with outer layer (left) and inner layer (right).