Supplementary Information File

Shockwave-Induced Structural Changes of Lipid Flat Disk and Transition to Vesicle

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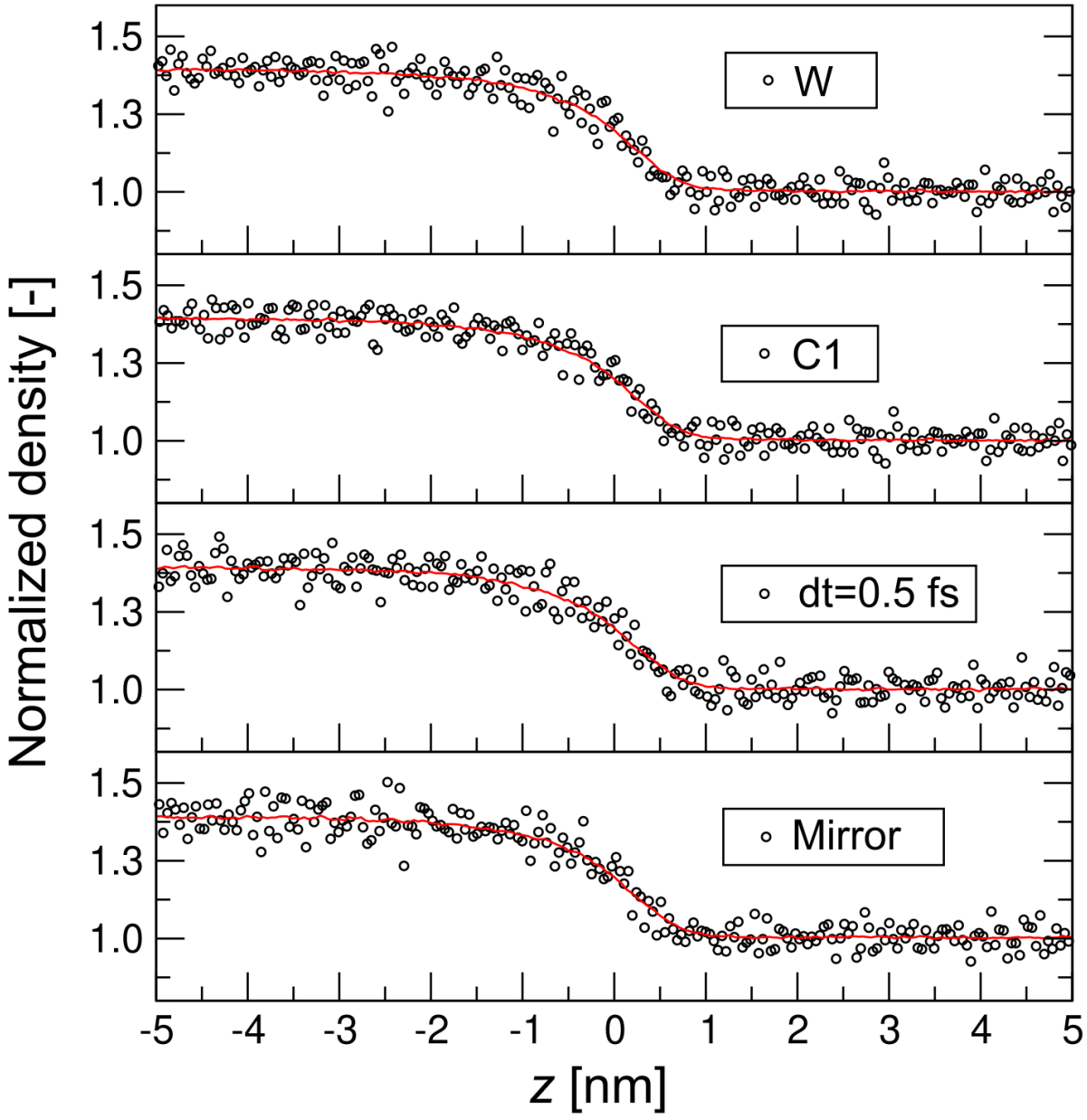

Figure S1 Density profiles of water beads across the shock for various piston-driven shockwave parameters and algorithms: the reference results labeled as “W”, with the C1 beads type for the wall atoms as “C1”, with the time step of 0.5 fs for integrating the equation of motion, as “dt=0.5fs” and with the momentum mirror algorithm using LAMMPS-like implementation as “Mirror”. The half of the density difference across the shock front is set to $z = 0$. The solid lines indicate moving averages for the eye guide. The densities are normalized by the averaged density at a temperature of 310 K and a pressure of 1 bar.

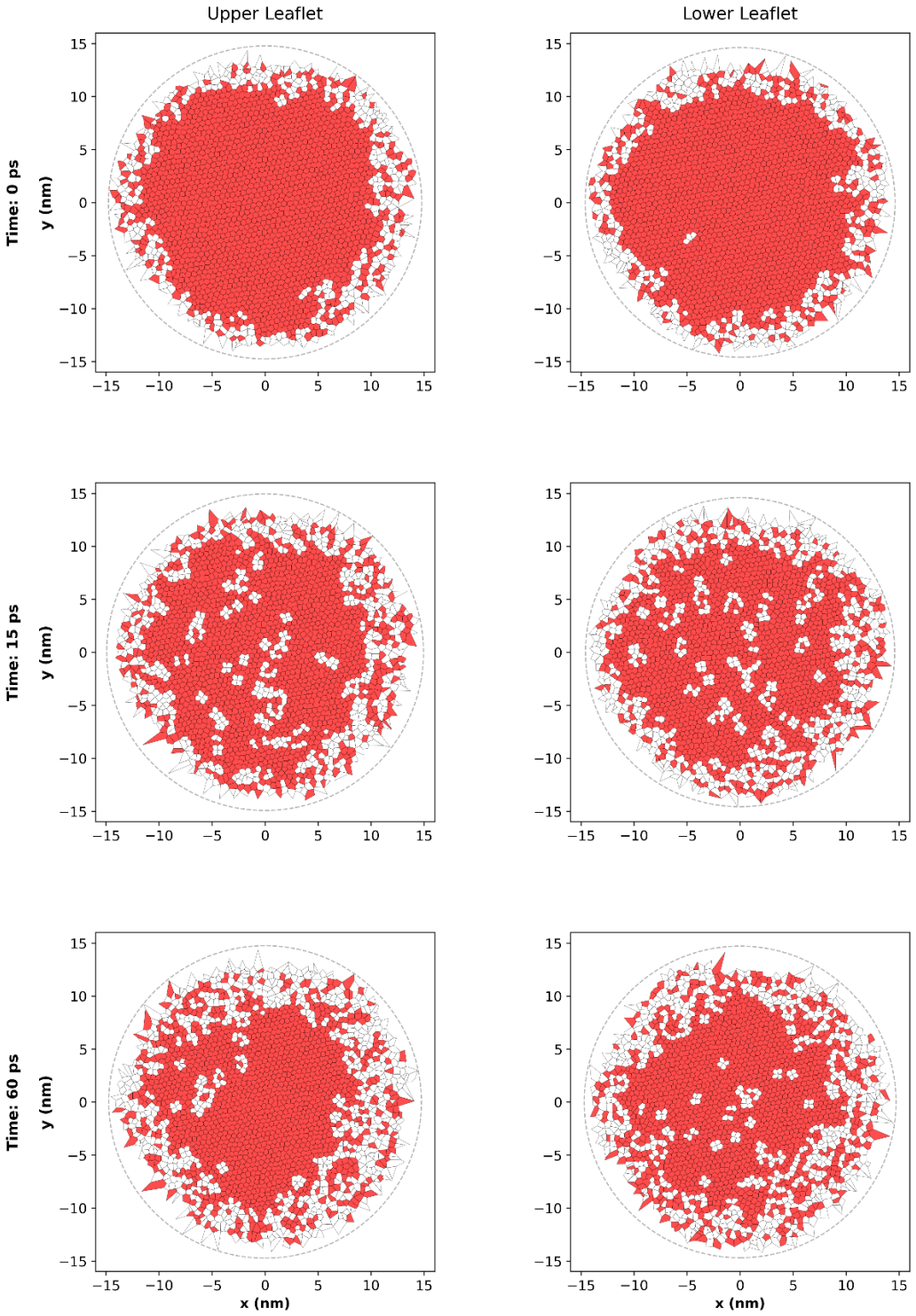

Figure S2 Representative results of the temporal changes in C2 bead distributions in the upper and lower leaflets of a lipid disk for $\theta = 0°$ and $U_p = 0.8$ km/s. The Voronoi tessellation is generated based on the positions of C2 beads, with the hexagonal Voronoi polygons highlighted in red. The dotted circle indicates the radius from the center of the disk to the outermost C2 bead positions, and polygons with vertices beyond this radius are not shown for clarity.

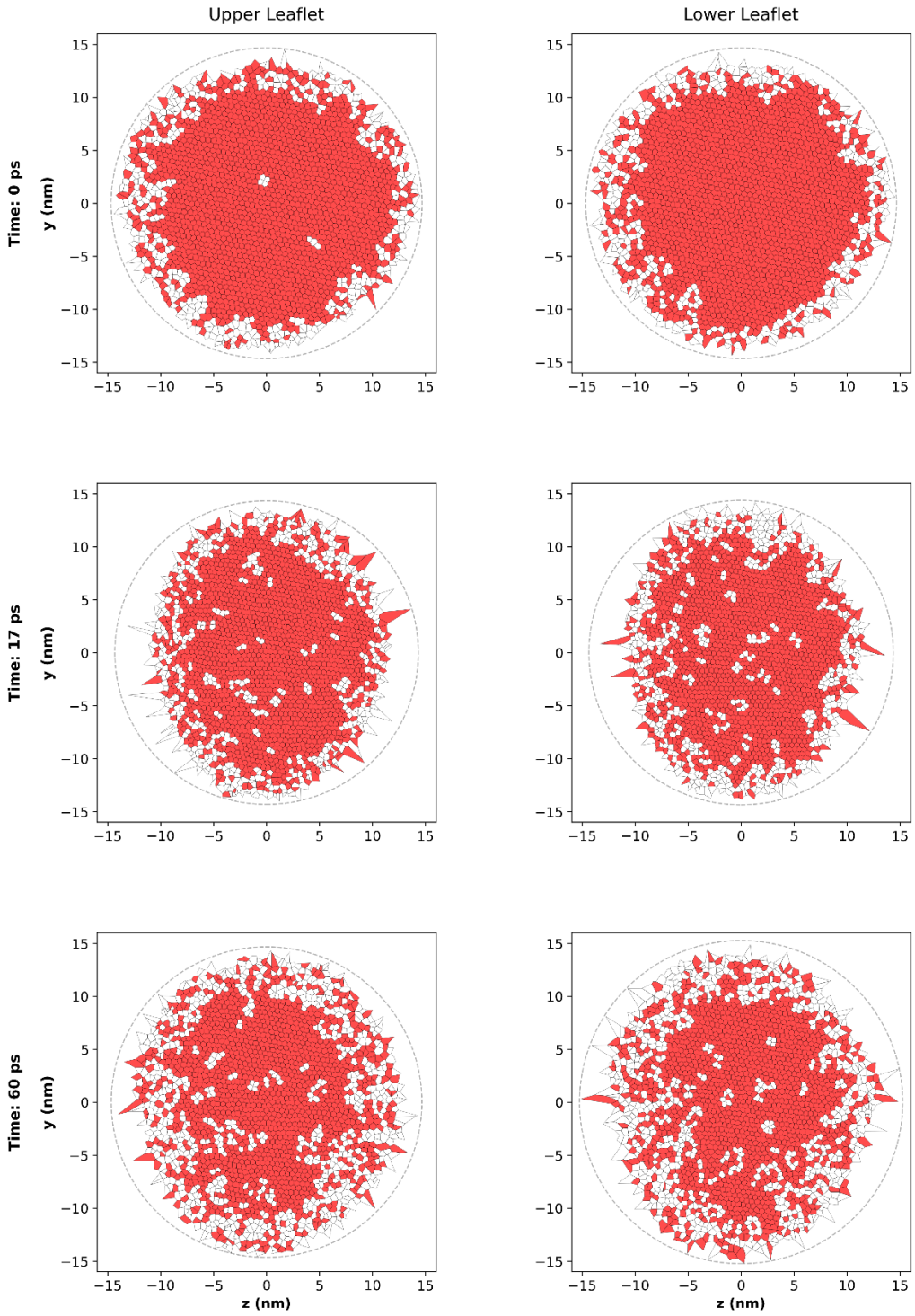

Figure S3 Representative results of the temporal changes in C2 bead distributions in the upper and lower leaflets of a lipid disk for $\theta = 90°$ and $U_p = 0.8$ km/s.

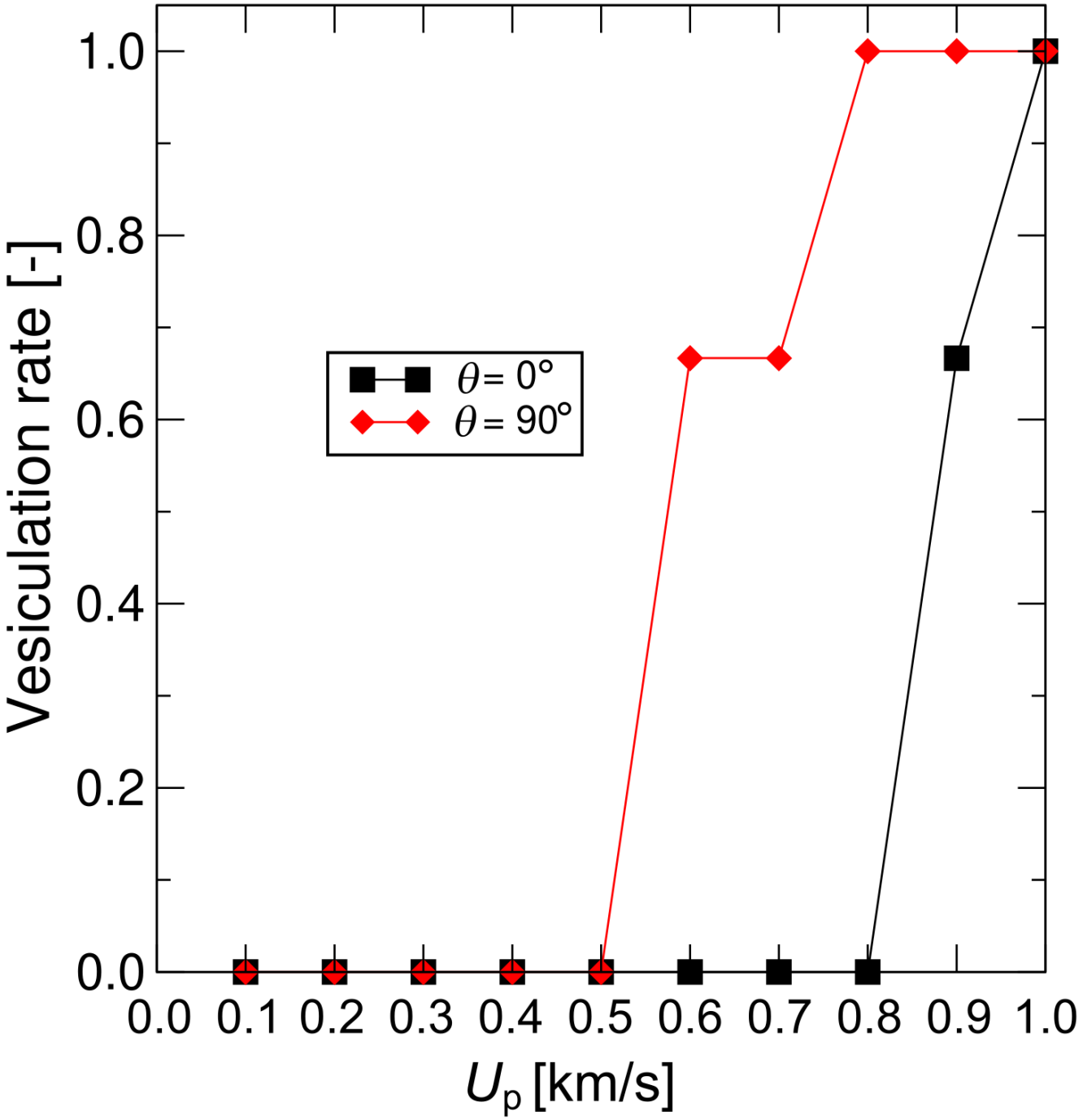

Figure S4 Vesiculation rate vs. U_p after the recovery MD simulations using the initial configurations of the fixed cut size.

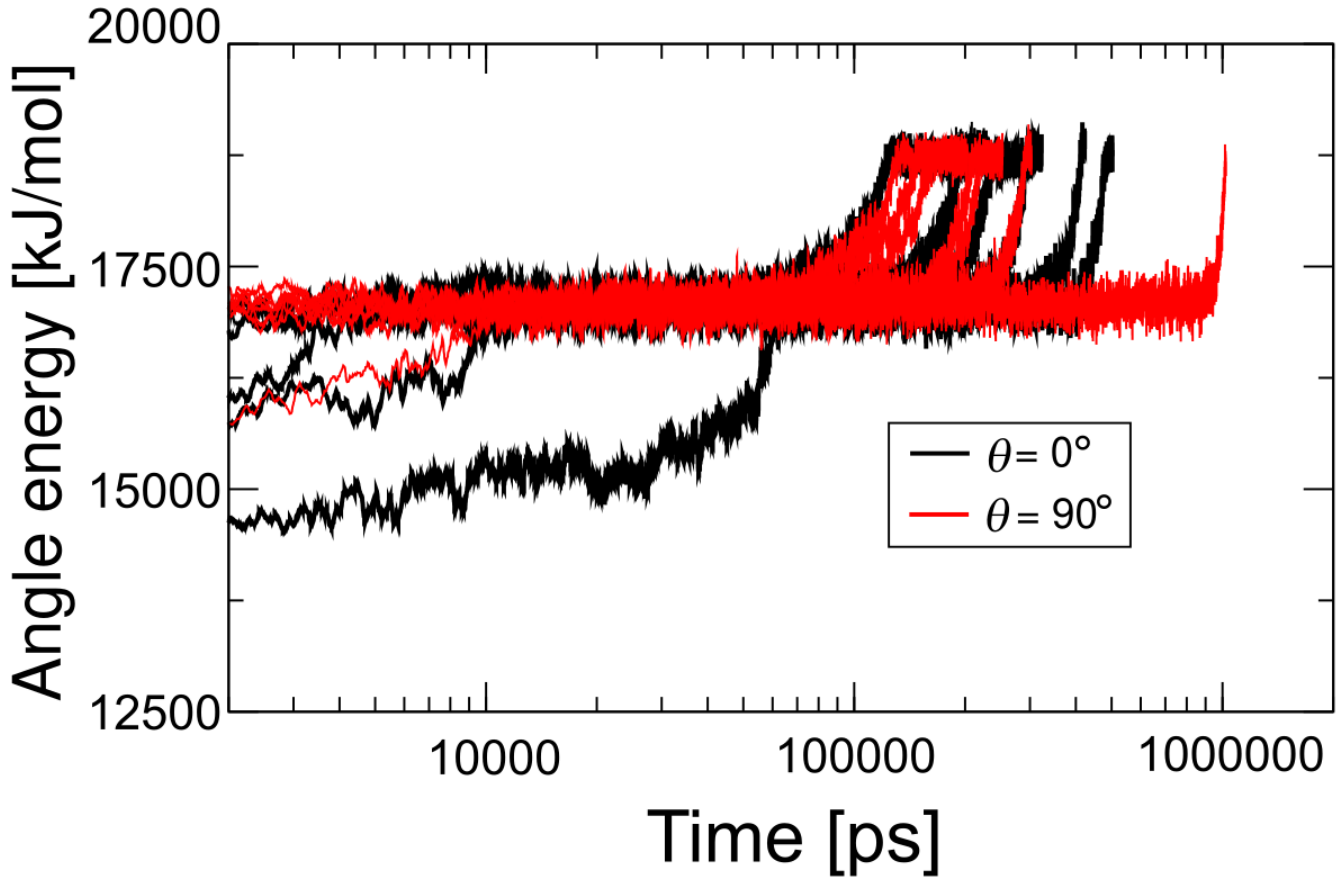

Figure S5 Temporal changes of angle potential energy for $\theta = 0°$ and $90°$ after the impact of shockwaves during vesiculation.