Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Lipid extraction mediates aggregation of carbon nanospheres in pulmonary surfactant monolayers

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The On-line Electronic Supplementary Information (ESI) includes two videos and nine figures:

Video S1: Lipid extraction dynamics by deposited CNS from PSM.

Video S2: Restrained lipid extraction under PSM compression.

Figure S1: Simulation system setup.

Figure S2: The surface tension of pure DPPC monolayer as a function of lipid area.

Figure S3: PSM perturbation by CNSs with different sizes.

Figure S4: Possible geometries of CNS aggregates.

Figure S5: Aggregation of CNSs with diameter of 3.0 nm under PSM compression.

Figure S6: Enhanced aggregation of CNSs with diameter of 1.0 nm under higher concentration

Figure S7: Evolution of pulling force energy departing two aggregated CNSs.

Figure S8: CNS cluster formation before contacting with PSM and subsequent insertion into PSM.

Figure S9: Interaction pathway between CNS with diameter of 3.0 nm and PSM with lipid area of 0.48 nm^2.

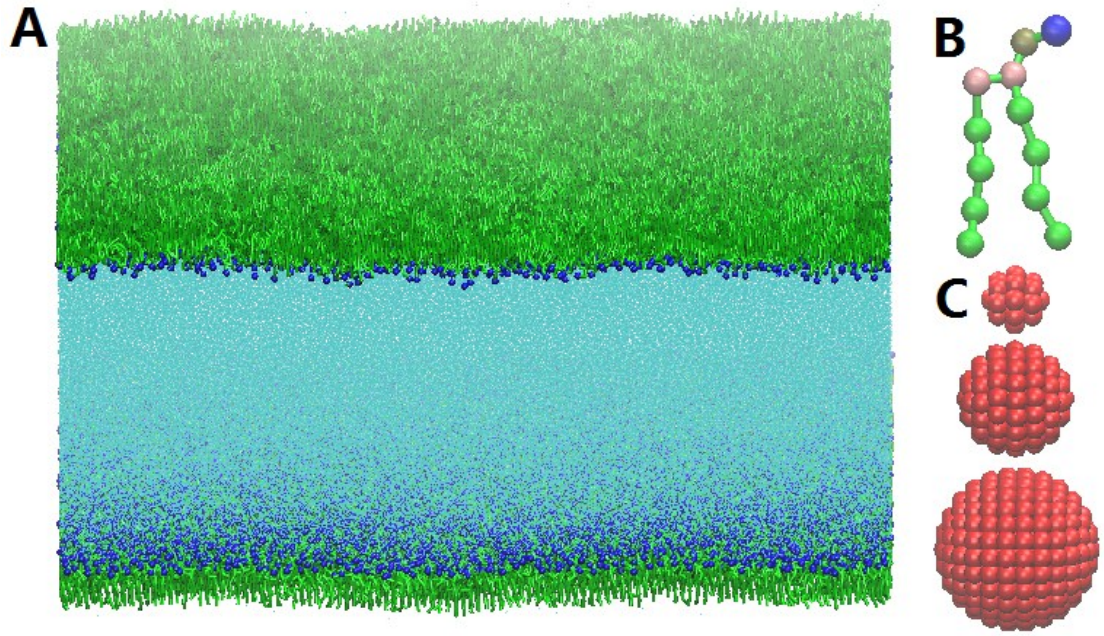

Fig. S1 A: Simulation system setup. A, bi-monolayer PSM model; B, DPPC lipid model; C, CNS model with diameters of 1 nm, 2 nm and 3 nm, respectively.

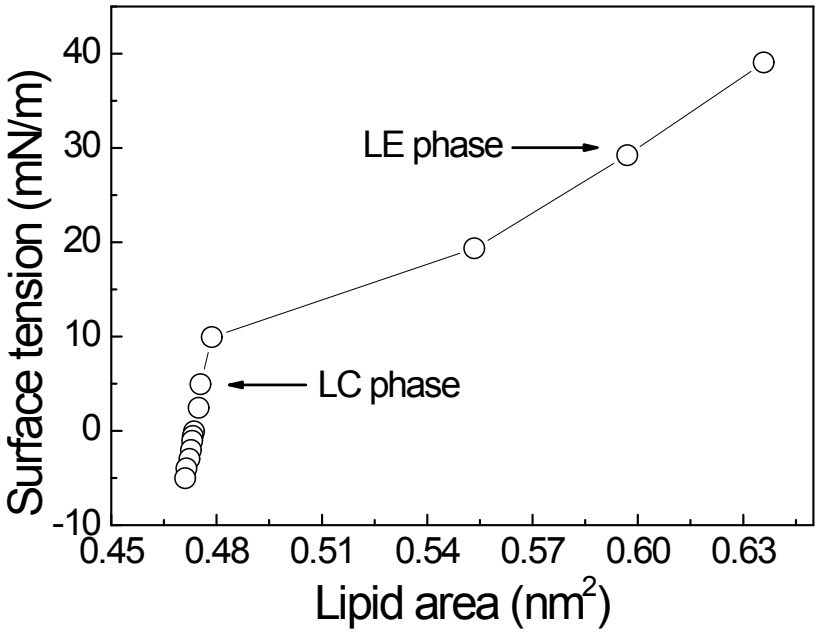

Fig. S2 The surface tension of pure DPPC monolayer as a function of lipid area.

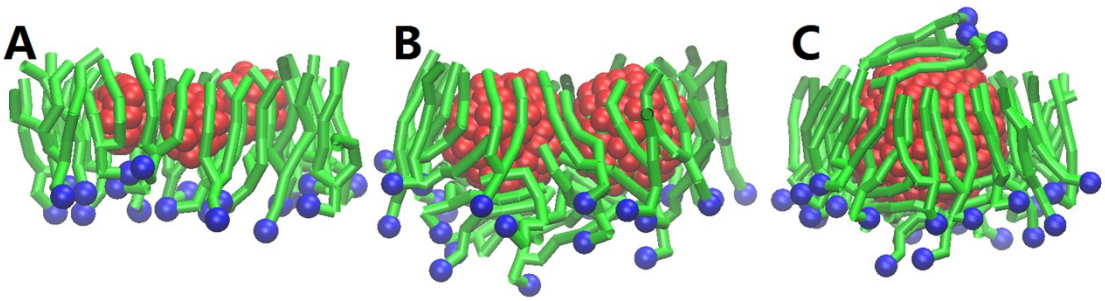

Fig. S3 PSM perturbation by CNSs with different sizes (A: D = 1.0 nm; B: D = 2.0 nm; C; D = 3.0 nm).

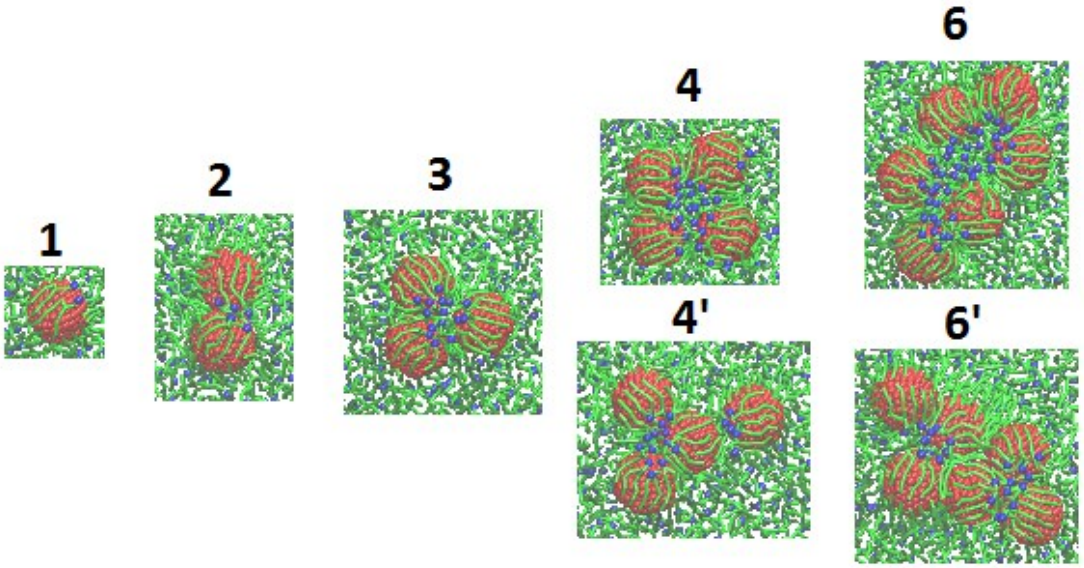

Fig. S4 Possible geometries of CNS aggregates and corresponding assembly way of extracted lipids.

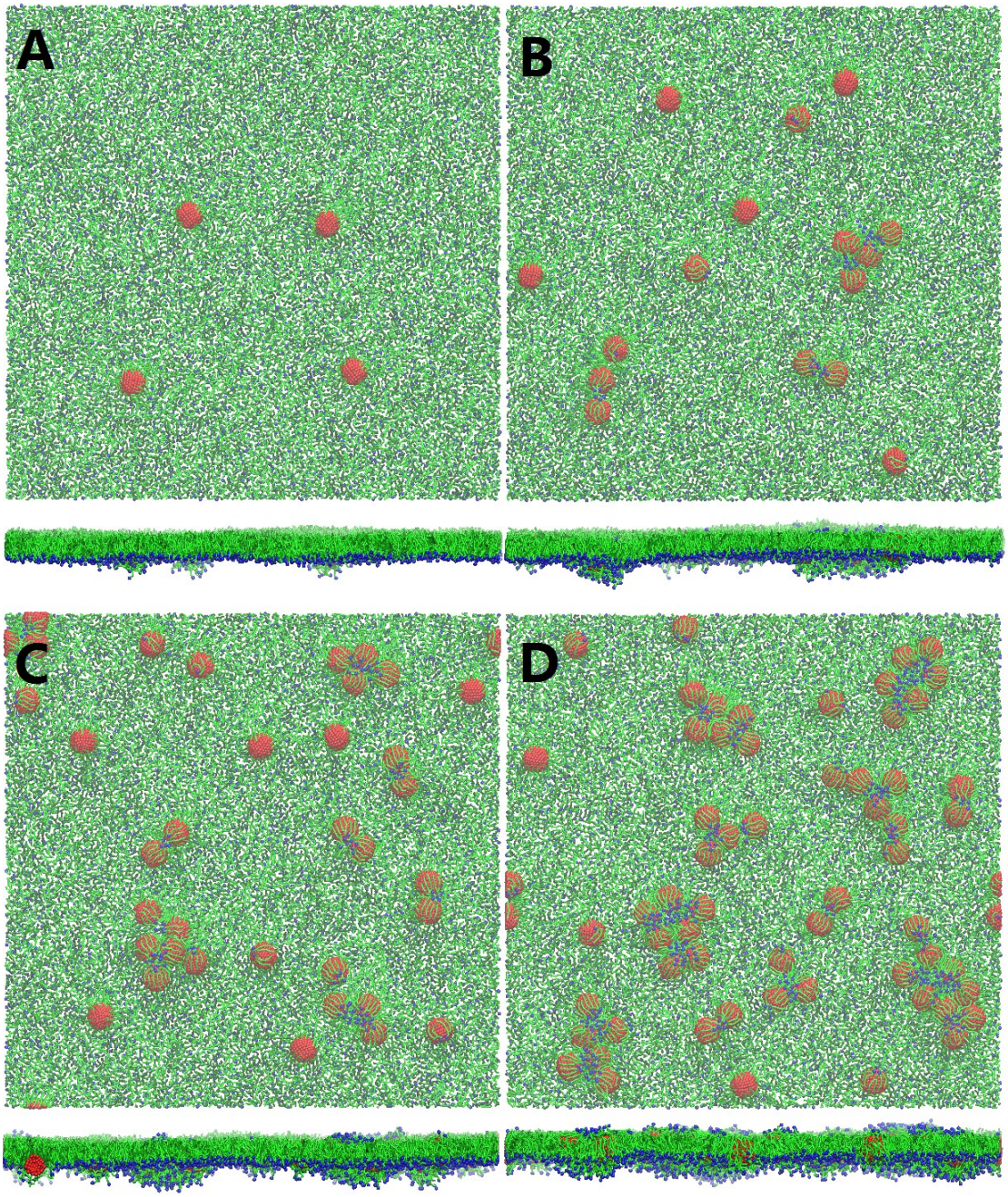

Fig. S5 Aggregation of CNSs with diameter of 3.0 nm and different [CNS]/[DPPC] ratios of 0.0008 (A), 0.003 (B), 0.0125 (C) and 0.02 (D). The area per lipid molecule was fixed to 0.55 nm^2, under which the PSM displays LE phase.

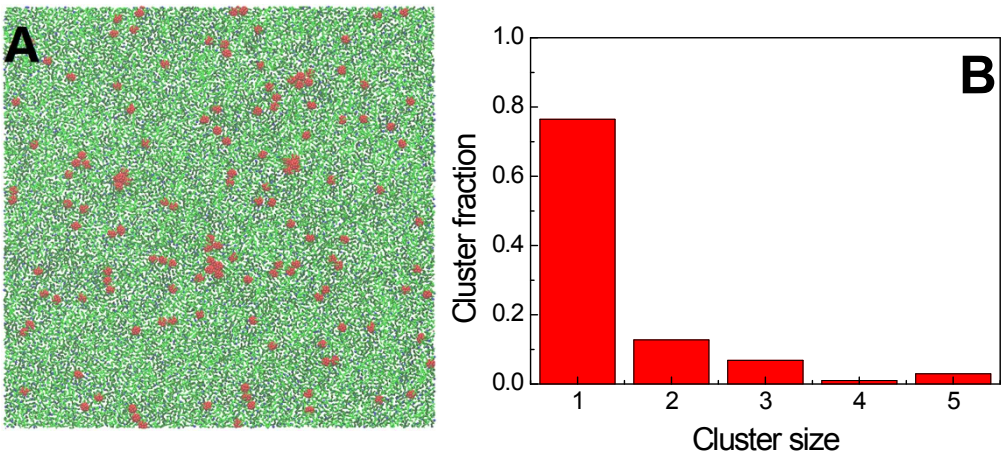

Fig. S6 Enhanced aggregation of CNSs with diameter of 1.0 nm under higher [CNS]/[DPPC] ratio of 0.03. The lipid area is fixed to 0.55 nm^2.

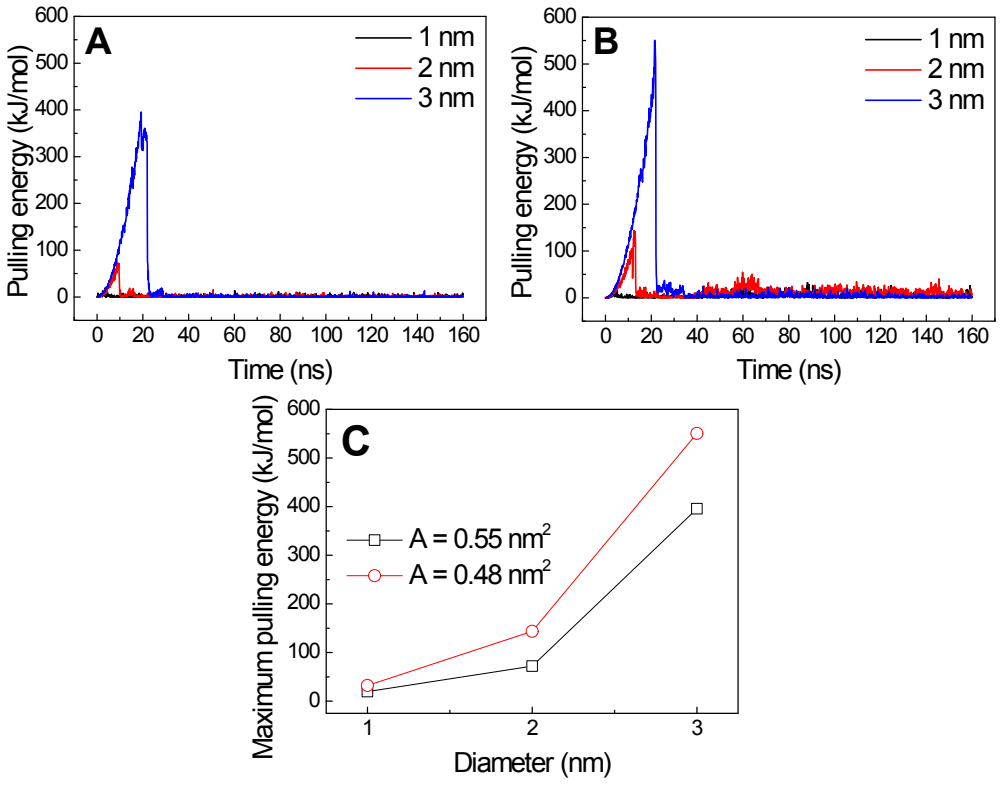

Fig. S7 Evolution of pulling force energy departing two aggregated CNSs under LE phase (A) and LC phase (B). C shows the maximum pulling energy for CNSs with different sizes and under different PSM tension.

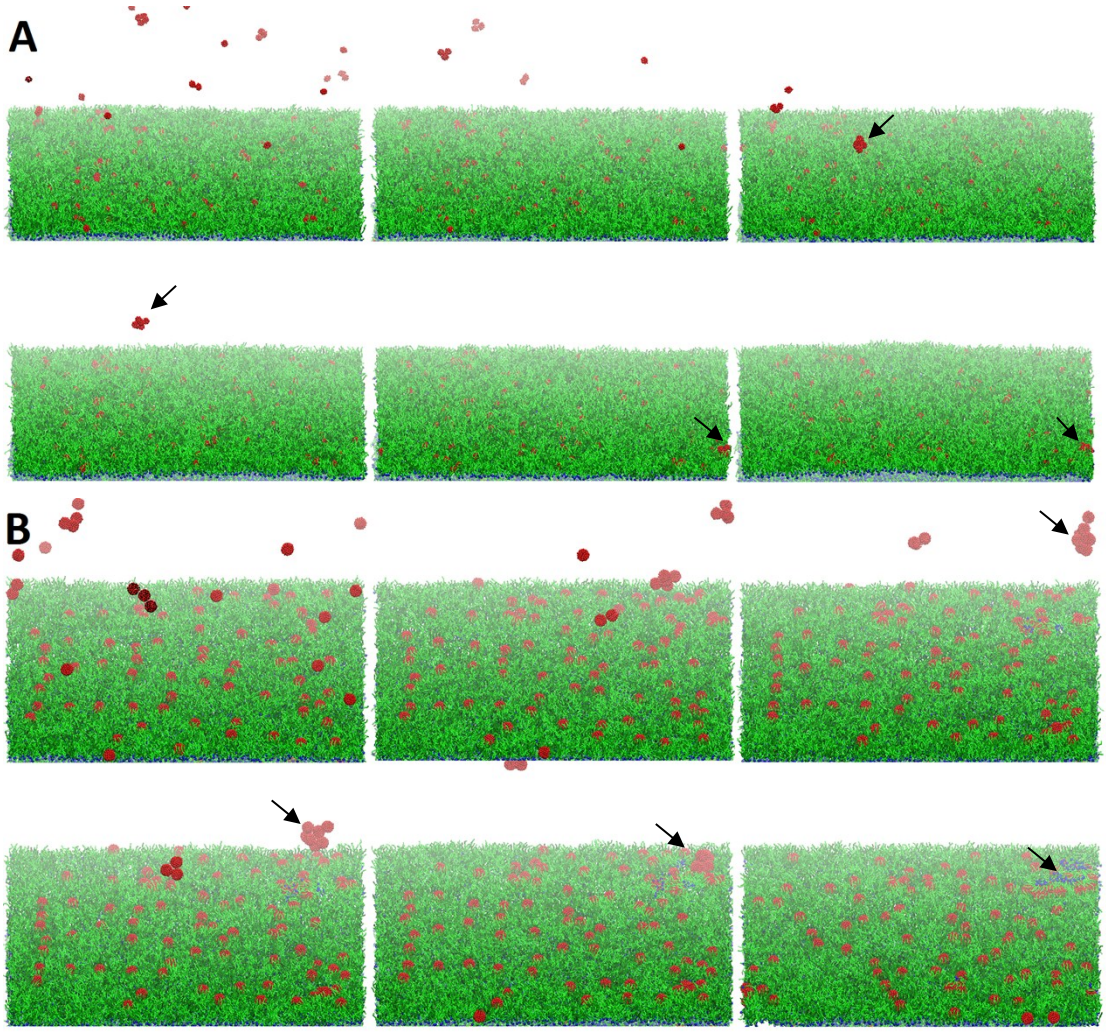

Fig. S8 CNS cluster formation before contacting with PSM and subsequent insertion into PSM. The CNS diameters were set to 1.0 nm (A) and 2.0 nm (B), respectively. The preformed CNS clusters were labeled by black arrows.

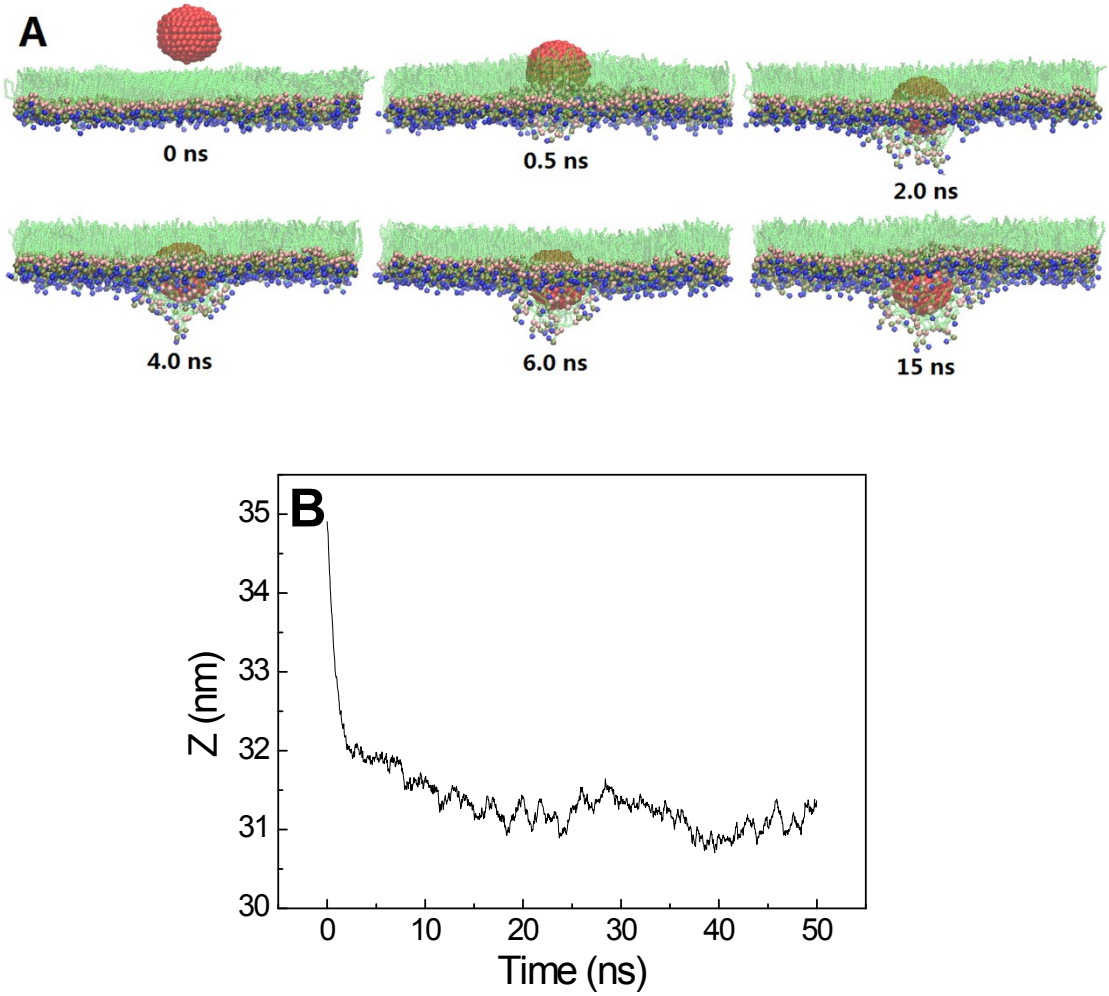

Fig. S9 Interaction between CNS with diameter of 3.0 nm and PSM with lipid area of 0.48 nm^2. A shows the interaction pathway and B shows the evolution of position of CNS along PSM normal direction.