Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supplementary information

Extracting pulmonary surfactants to form inverse micelles on suspending graphene nanosheets

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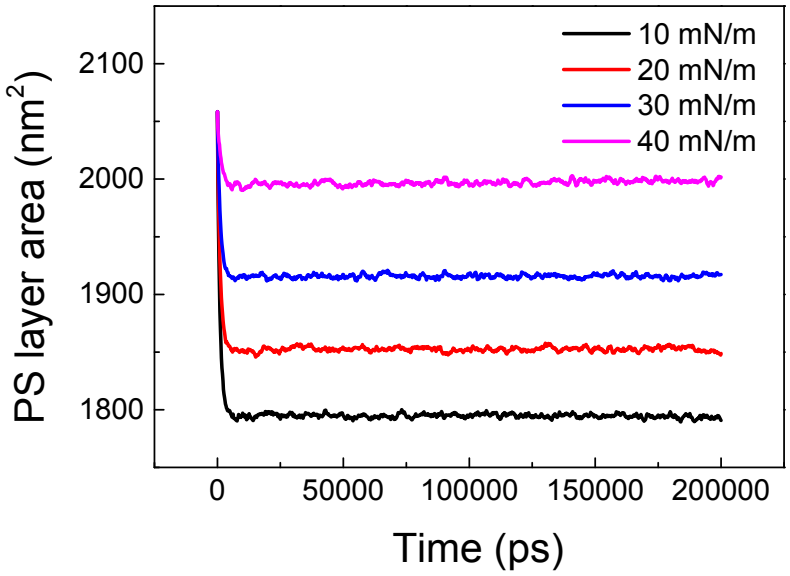

Fig. S1 Time evolutions of the PS layer area under different surface tensions.

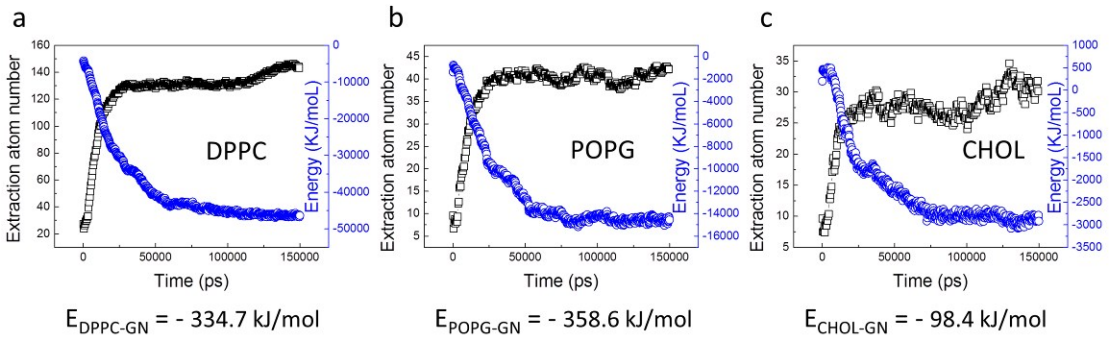

Fig. S2 Time evolutions of the extraction numbers and the interaction energy for three different PS molecules, including DPPC, POPG and cholesterol. The averaged interaction energy per PS molecule was given in the lower side, showing much higher binding strength for DPPC and POPG molecules.

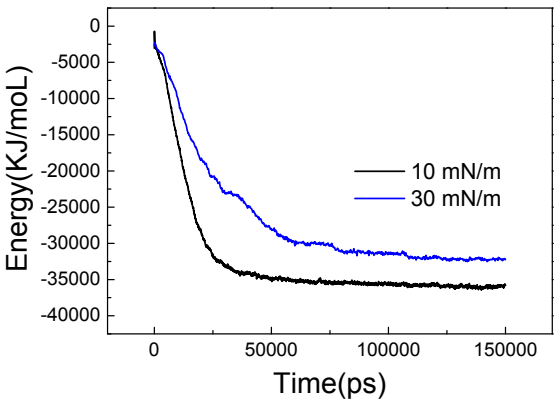

Fig. S3 Time evolutions of interaction energy between GN and PS molecules under surface tensions of 10 mN/m and 30 mN/m.

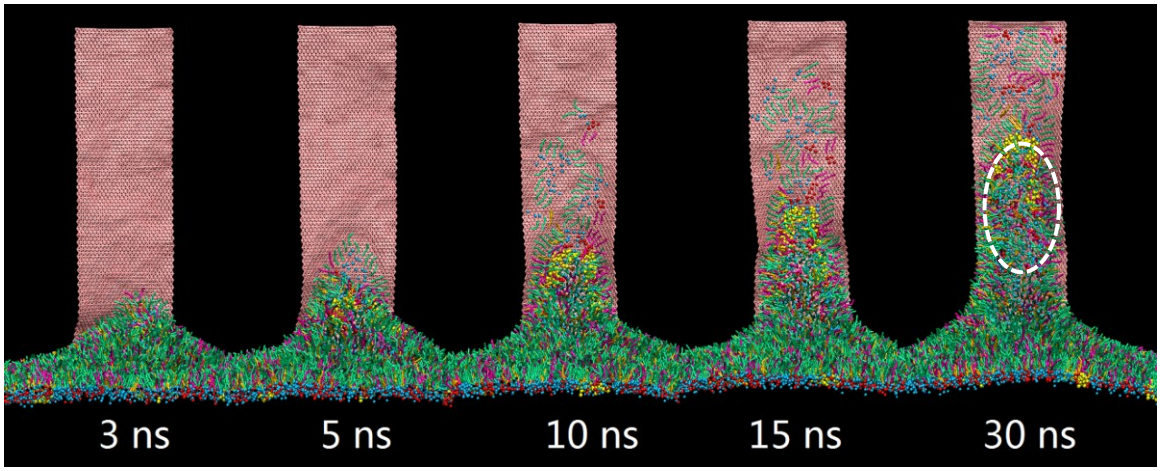

Fig. S4 Enhanced PS extraction under lower surface tension of 10 mN/m. One SP-C protein being extracted from the layer is marked by a write dashed circle.

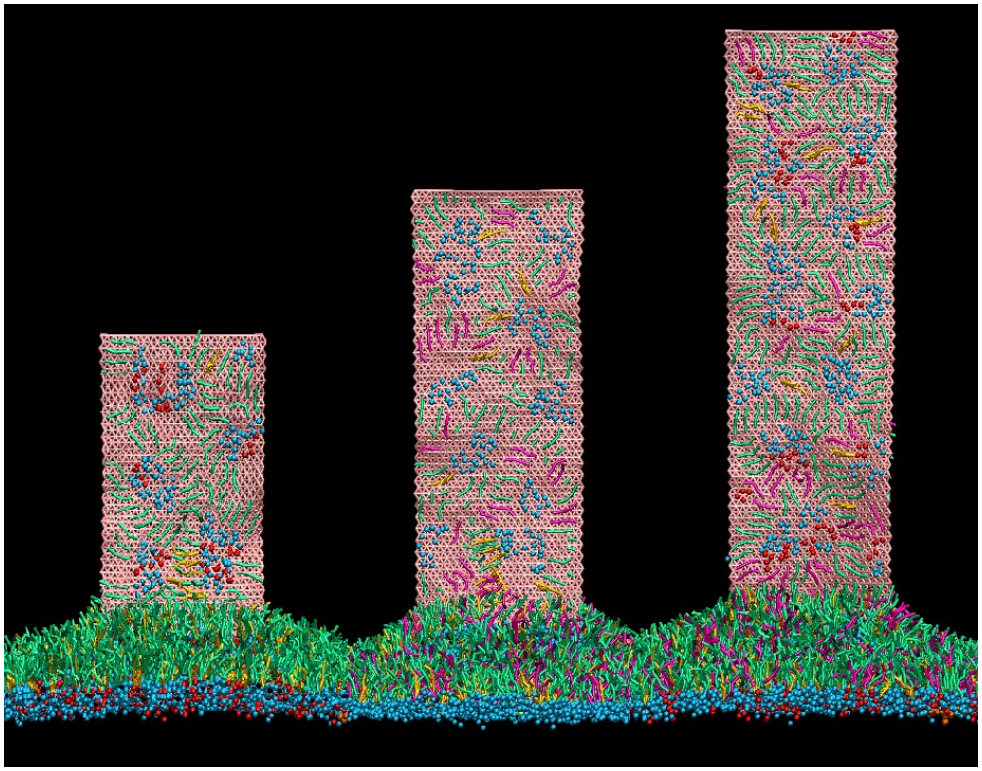

Fig. S5 Final snapshots illustrating the effect of GN size on the PS extraction.

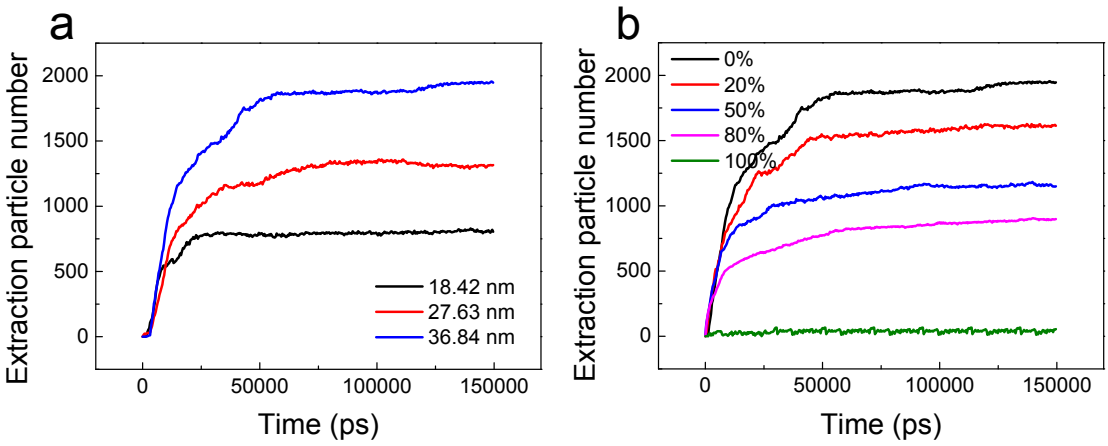

Fig. S6 The effects of GN size and oxidation ratio on the PS extraction. (a) Time evolutions of extraction particle number by three GNs with the same width but different lengths. (b) Time evolutions of extraction particle number by five GNs with the same lateral size but different oxidation ratios.

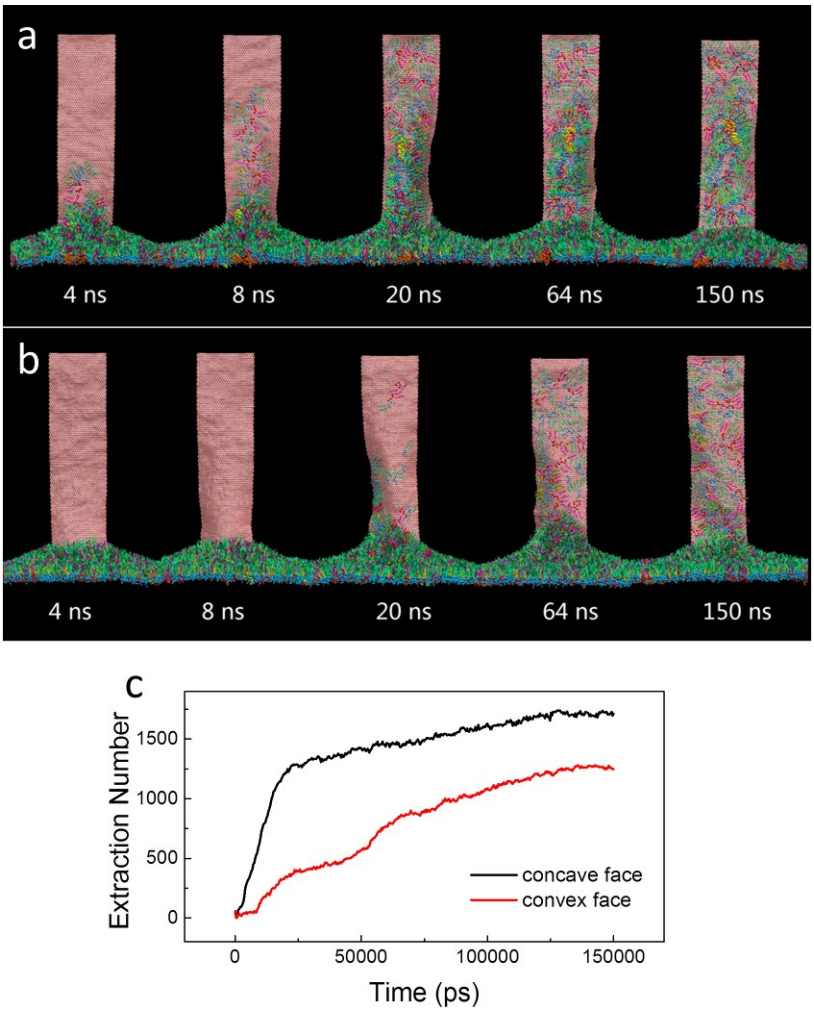

Fig. S7 Asynchronous extraction of PS molecules by two surfaces of a curved GN. (a) PS extraction process on the concave GN surface. (b) PS extraction process on the convex GN surface. (c) Time evolutions of the extraction number on both surfaces.

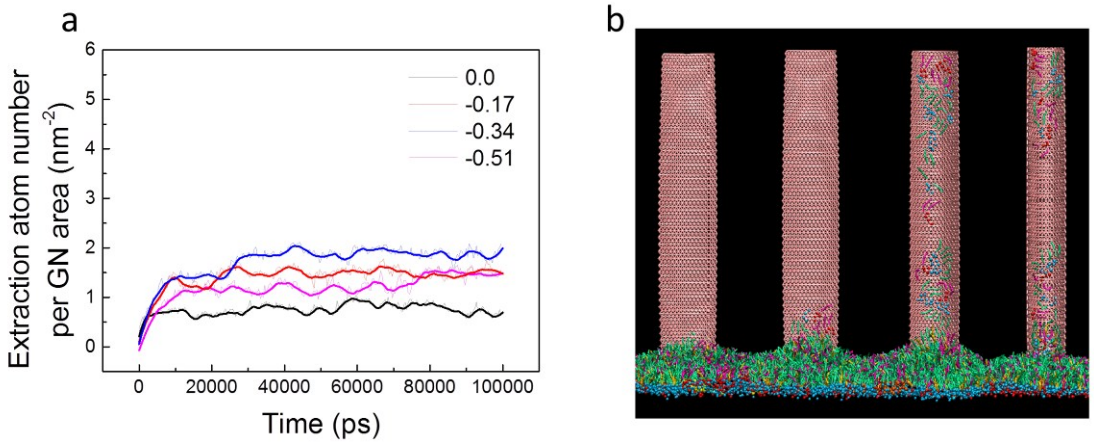

Fig. S8 (a) Time evolutions of the extraction atom number for GNs having a decreased width of 5.5 nm and different curvatures. (b) Final snapshots for PS extraction on four curved GNs.

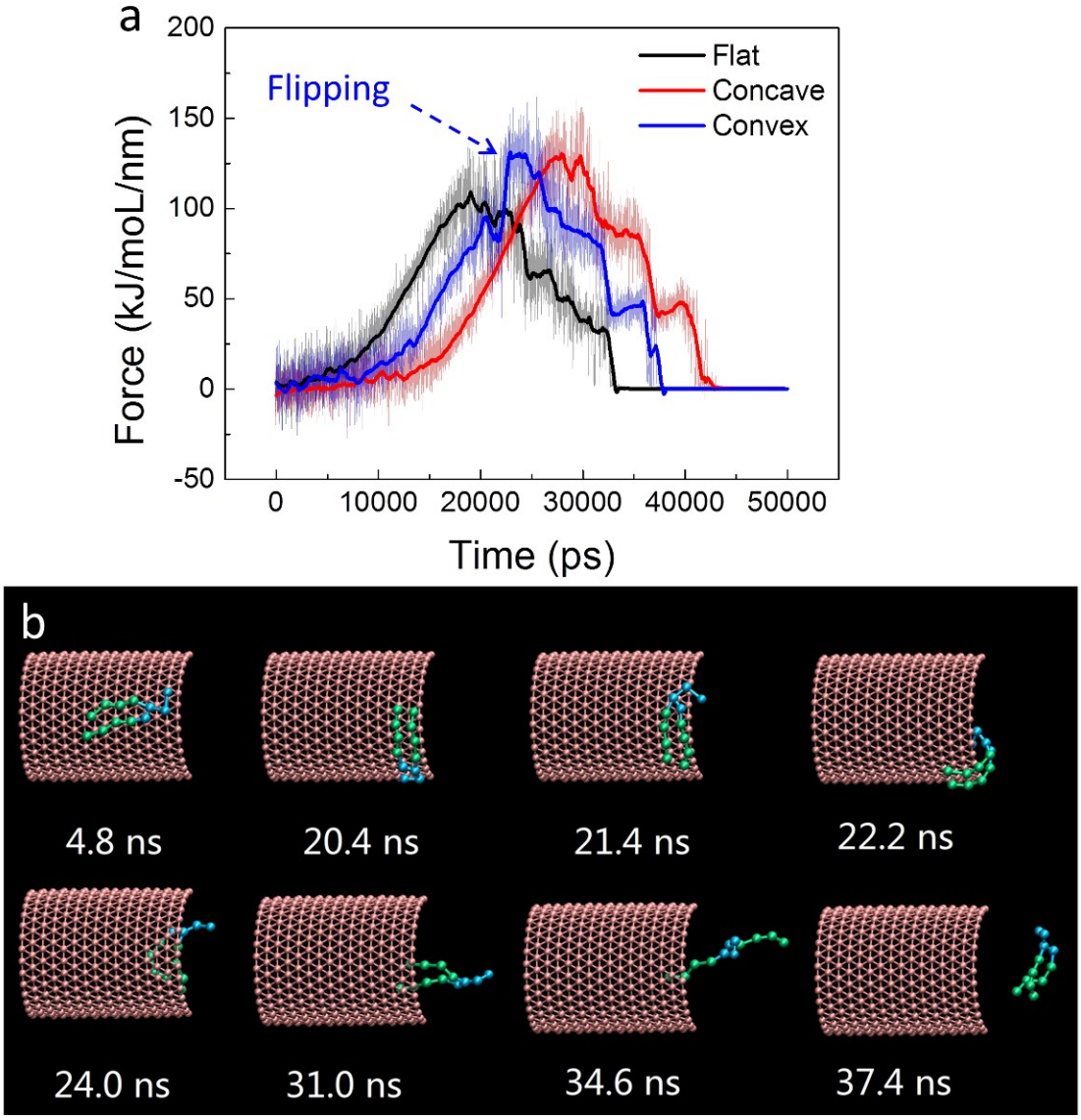

Fig. S9 (a) Evolutions of pulling force exerted on lipid along surfaces of GNs with zero (flat), positive (concave) and negative (convex) curvatures. (b) Time sequence of typical snapshots showing he conformational change of lipid along convex GN surface.

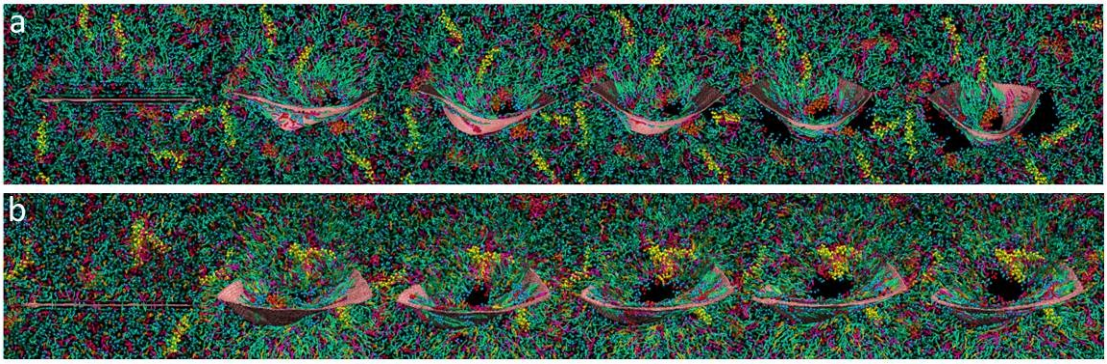

Fig. S10 PS layer rupture under higher tensions of 30 mN/m (a) and 10 mN/m (b) by enhanced PS extraction on a larger GN (36.8 nm × 18.4 nm).

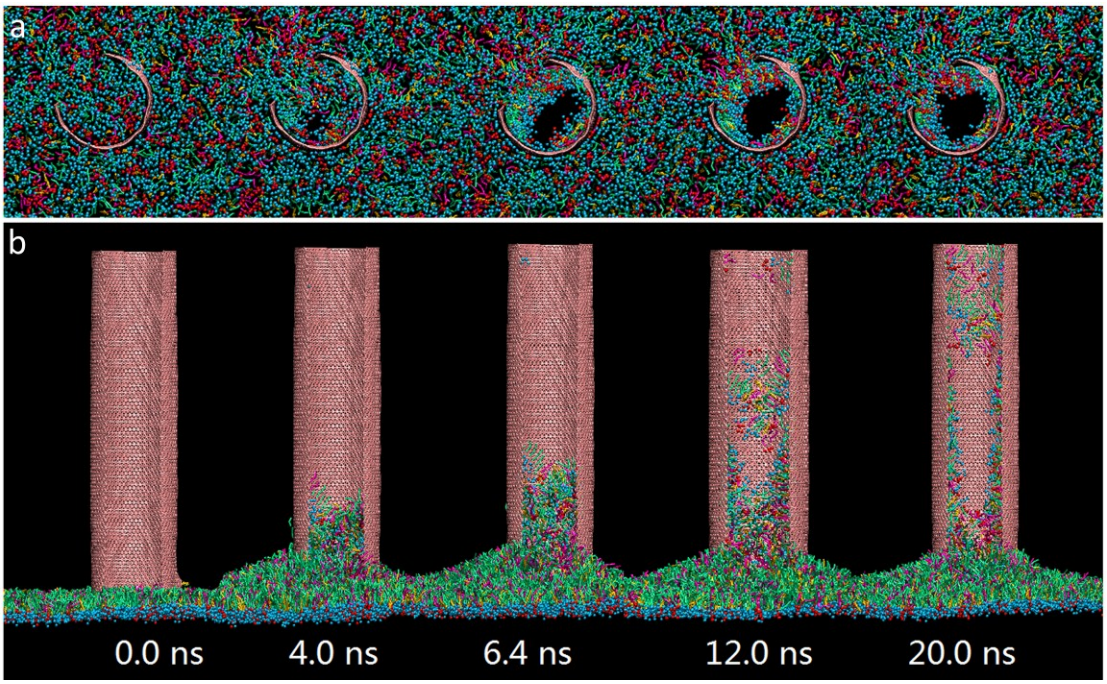

Fig. S11 PS layer poration inside a curved GN. (a) The detailed poration process from the top view. (b) The side view gives the enhanced PS extraction from the inner GN surface.

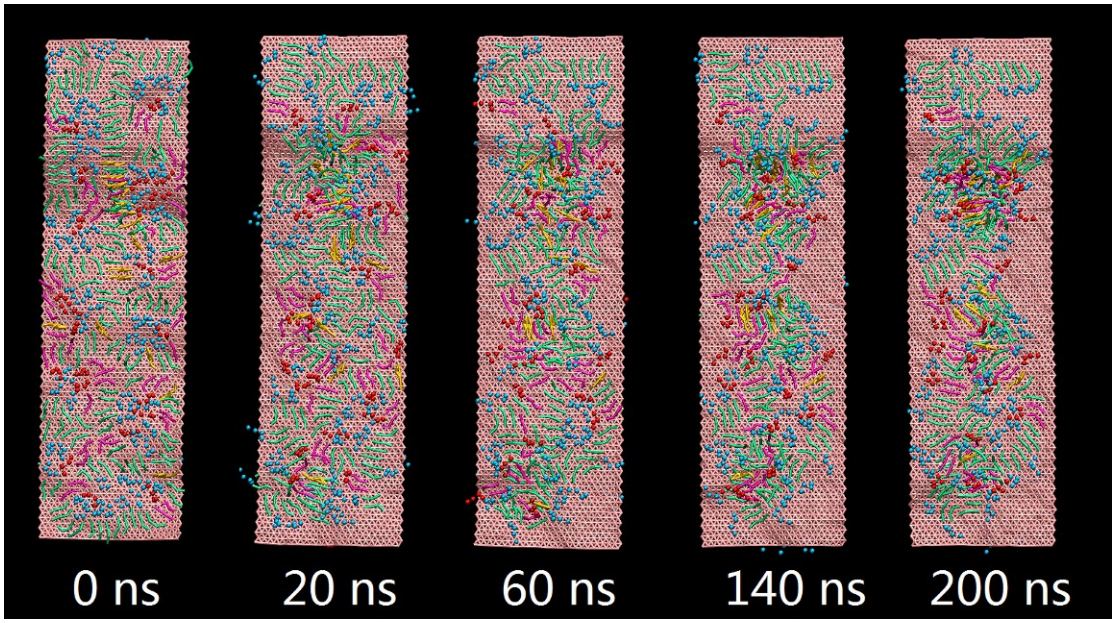

Fig. S12 Structural evolution of the PS-GN complex when being transferred into the water phase.