Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information:

The role of size and nature in nanoparticle binding to a model lung membrane: an atomistic study.

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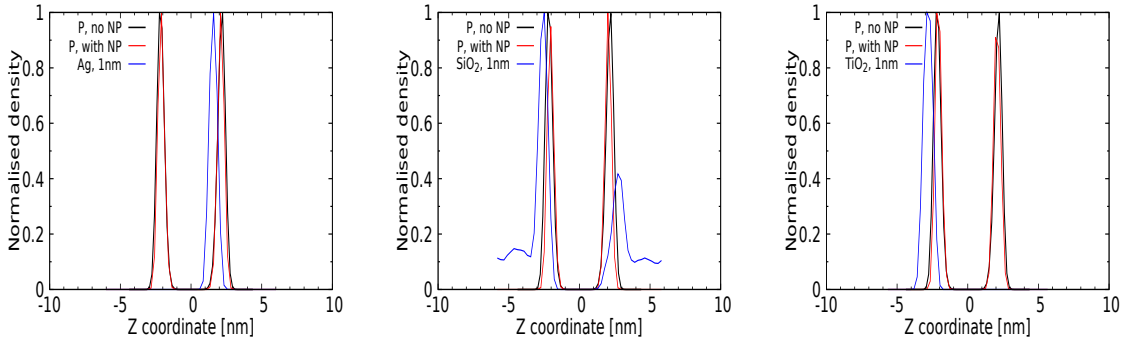

Figure S1: Normalized density profiles for the phosphor group of the DPPC, DOPC and POPC lipids in the bilayer (black line without a NP; red line with NP) and for the 1 nm NP itself (blue solid line): Ag(left), SiO_2(middle), and TiO_2(right). The origin is selected to correspond to the center of the lipid bilayer. Profiles were calculated from simulation data for the last 100 ns of a 400 ns production run, and obtained as an average over all lipids in both leaflets.

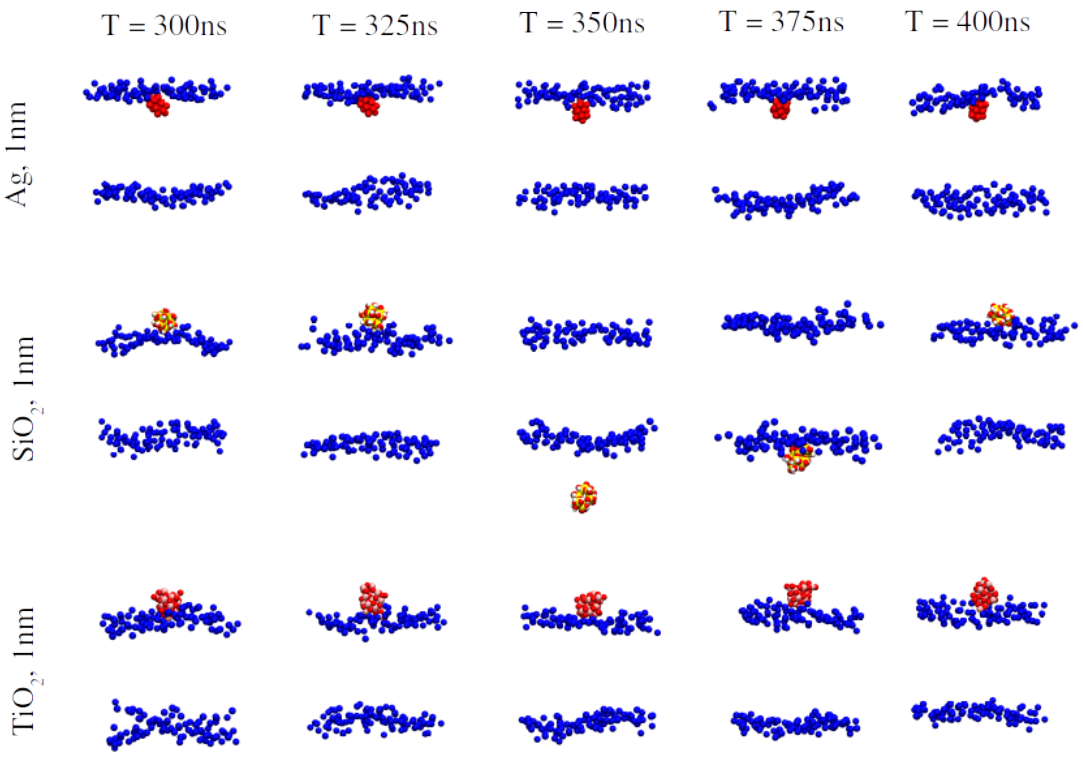

Figure S2: Orthogonal projections of simulation snapshots at selected time steps T for systems containing a 1 nm of Ag (top), SiO_2 (middle), and TiO_2 (bottom) NP illustrating the partial wrapping. As the nature of the lipids is not important at this stage, phosphorus and nitrogen atoms in DPPC, DOPC, and POPC are shown as blue spheres, and all other atom types are omitted for clarity. The Ag atoms in the NPs are shown as red spheres, while Si, Ti, and oxygen atoms are in yellow, pink, and red sphere respectively. As indicated, snapshots were generated at 25 ns intervals from the last 100 ns of a 400 ns production run.

Table S1: Average area per lipid (nm^2) for pure bilayer and in the presence of three NP: Ag, SiO_2, and TiO_2 for three different diameters d (1 nm, 3 nm and 5 nm). Analysis for individual cases was performed using the last 100 ns of 400 ns production run. The standard error for all the average values are also shown.

NP	d (nm)	DPPC	DOPC	POPC	CHOL
No NP	-	0.56 ± 0.013	0.59 ± 0.023	0.59 ± 0.021	0.28 ± 0.020
	1	0.57 ± 0.020	0.59 ± 0.034	0.57 ± 0.034	0.28 ± 0.032
Ag	3	0.49 ± 0.057	0.47 ± 0.041	0.55 ± 0.057	0.28 ± 0.022
	5	0.49 ± 0.094	0.50 ± 0.074	0.46 ± 0.092	0.23 ± 0.046
	1	0.57 ± 0.020	0.59 ± 0.036	0.59 ± 0.033	0.29 ± 0.033
SiO_2	3	0.50 ± 0.023	0.53 ± 0.033	0.54 ± 0.032	0.28 ± 0.022
	5	0.52 ± 0.015	0.57 ± 0.028	0.52 ± 0.037	0.26 ± 0.014
	1	0.57 ± 0.019	0.58 ± 0.032	0.58 ± 0.033	0.26 ± 0.033
TiO_2	3	0.51 ± 3.150	0.58 ± 0.036	0.50 ± 0.047	0.27 ± 0.020
	5	0.53 ± 1.780	0.54 ± 0.025	0.53 ± 0.030	0.23 ± 0.028

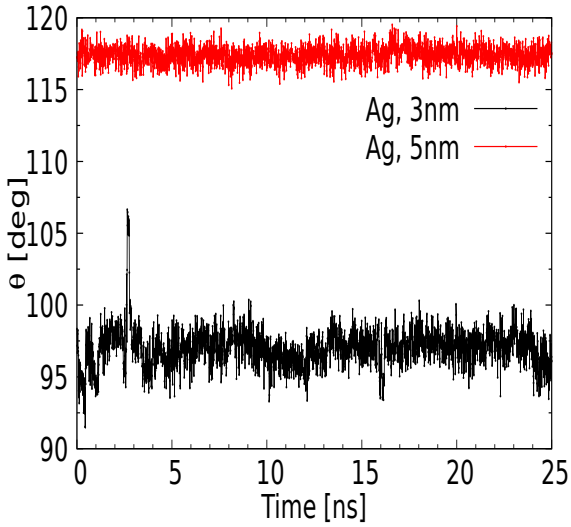

Figure S3: Time evolution of contact angle for 3 nm Ag NP (black line) and 5 nm Ag NP (red line).The contact angle, θ, is the wrapping angle defined in earlier studies.[1] It is defined as the angle between the membrane normal and the vector connecting the center of the NP and the contact ring where the lipid bilayer detaches from the NP.

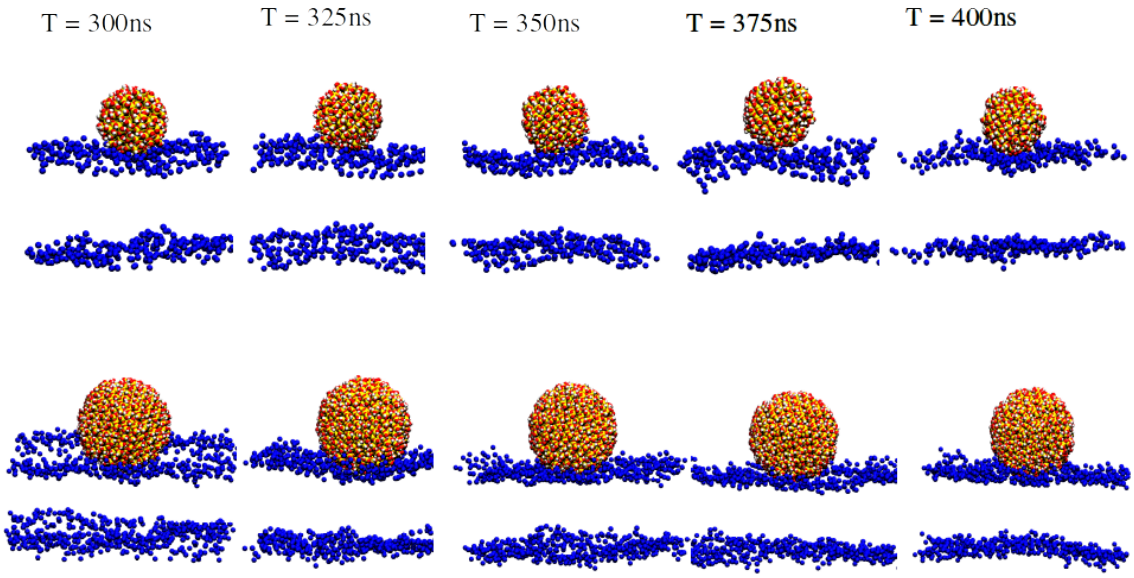

Figure S4: Orthogonal projections of simulation snapshots at selected time steps T for systems containing a 3 nm SiO_2 (top) and 5 nm SiO_2 (bottom) NP illustrating the bound state. As the nature of the lipids is not important at this stage, phosphorus and nitrogen atoms in DPPC, DOPC, and POPC are shown as blue spheres, and all other atom types are omitted for clarity. The silicon, oxygen, and hydrogen atoms in the NPs are shown as yellow, red, and white spheres. As indicated, snapshots were generated at 25 ns intervals from the last 100 ns of a 400 ns production run.

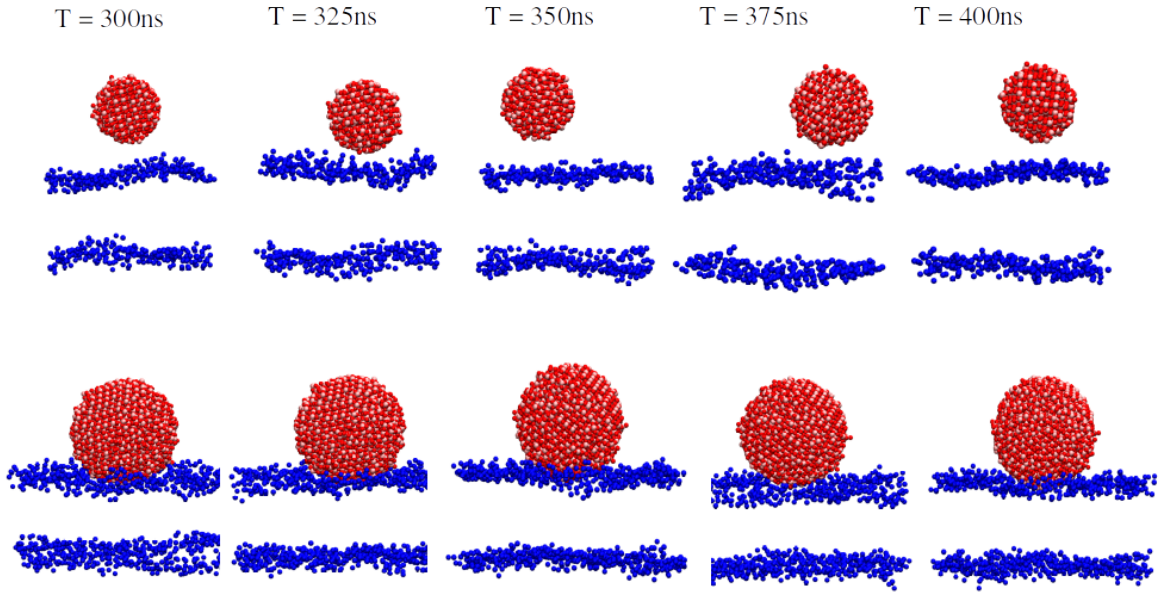

Figure S5: Orthogonal projections of simulation snapshots at selected time steps T for systems containing a 3 nm TiO_2 (top) and 5 nm TiO_2 (bottom) NP illustrating the (un) bound state. As the nature of the lipids is not important at this stage, phosphorus and nitrogen atoms in DPPC, DOPC, and POPC are shown as blue spheres, and all other atom types are omitted for clarity. The titanium and oxygen atoms in the NPs are shown as pink and red spheres. As indicated, snapshots were generated at 25 ns intervals from the last 100 ns of a 400 ns production run.

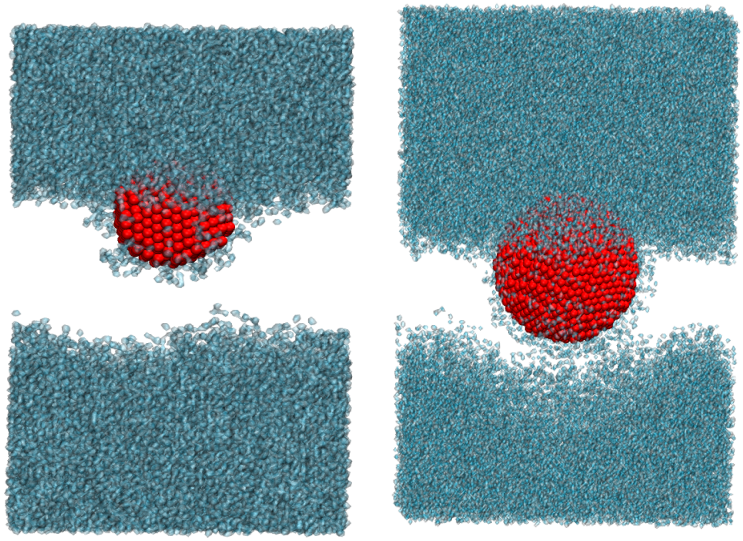

Figure S6: Final simulation snapshots of Ag 3 nm (left) and 5 nm (right) NP. The membrane constituents have been removed to focus on the water content. The Ag atoms in the Ag NP are shown as red spheres, while the water is shown as blue beads.

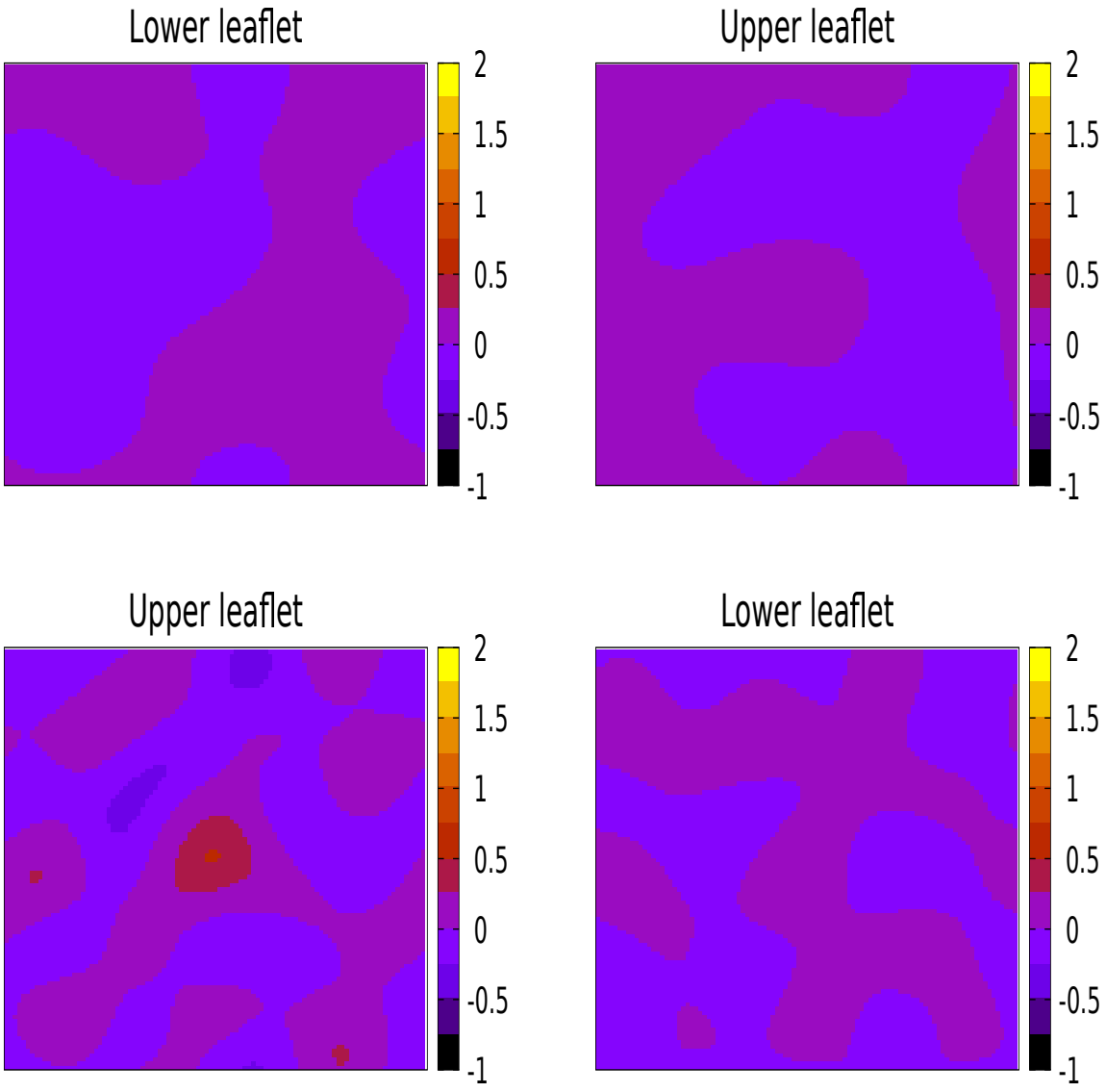

Figure S7: The mean curvature induced by a SiO_2 NP 3 nm (top) and 5 nm (bottom) in a lipid bilayer comprised of DPPC:DOPC:POPC:CHOL in 5:2:2:1 proportion. We applied a band pass filter with $q_{low} = 0.5$ nm^{-1} and $q_{high} = 2.0$ nm^{-1}. Local curvatures were obtained by the program "g lomepro".

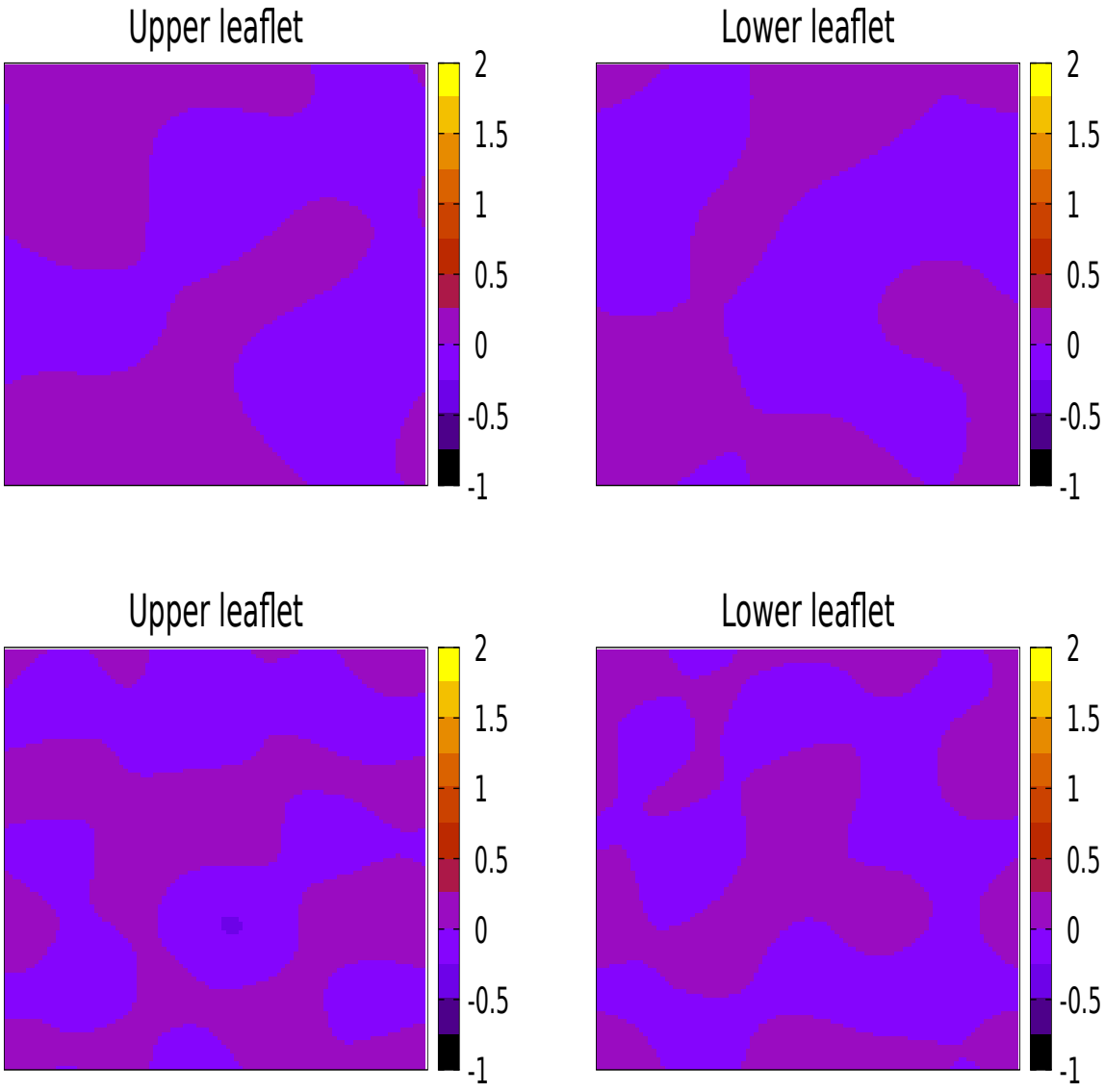

Figure S8: The mean curvature induced by a TiO_2 NP 3 nm (top) and 5 nm (bottom) in a lipid bilayer comprised of DPPC:DOPC:POPC:CHOL in 5:2:2:1 proportion.We applied a band pass filter with $q_{low} = 0.5$ nm^{-1} and $q_{high} = 2.0$ nm^{-1}. Local curvatures were obtained by the program "g lomepro".

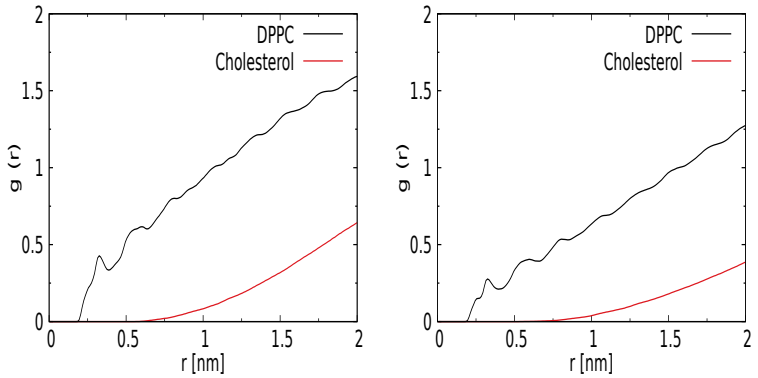

Figure S9: Radial distribution function of 3 nm (left) and 5 nm (right) Ag NP with DPPC (black) and cholesterol (red). The RDFs considered the last 100 ns of a 400 ns production run and all lipids in both leaflets. We used the molecular centers of mass to calculate the RDFs.

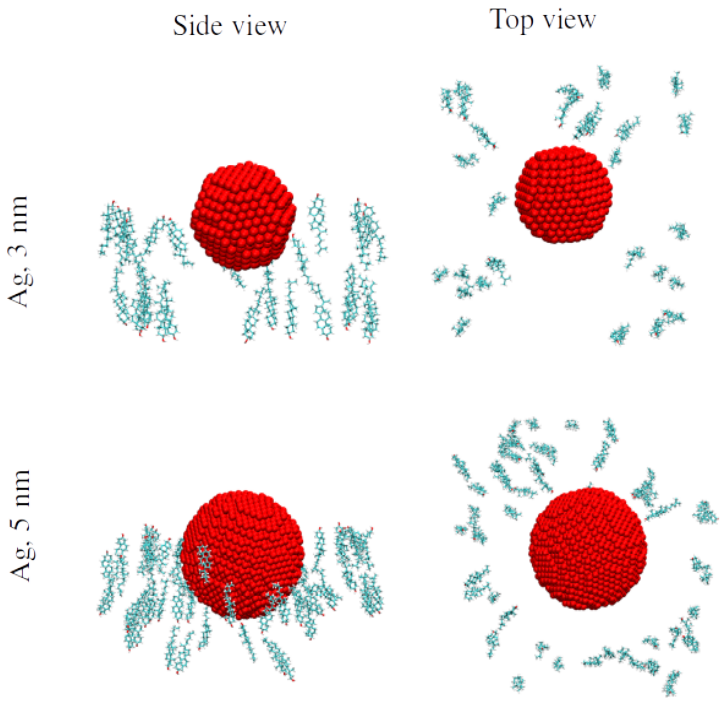

Figure S10: Side (left) and top (right) view for the cholesterol content of the membrane and the Ag NP. All other constituent are not shown. For all the cholesterol molecules, the carbon, oxygen, and hydrogen are shown in stick representation in blue, red, and white color respectively. The Ag atoms are shown as red spheres.

References

(1) E. J. Spangler, S. Upreti and M. Laradji, *The Journal of chemical physics*, 2016, **144**, 044901.