Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Nanoparticle translocation through a lipid bilayer tuned by surface chemistry†

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Supporting Information

1. Snapshots of nanoparticles with 15 and 25% of charge

Simulations using nanoparticles with 15 and 25% of charge also were performed to ensure the capacity of low charge densities to favor membrane penetration compared to nanoparticles with 40, 60, 80 and 100% of charge. As can be noticed, Figure S1 revealed that the results are in agreement with nanoparticles with 20% of charge.

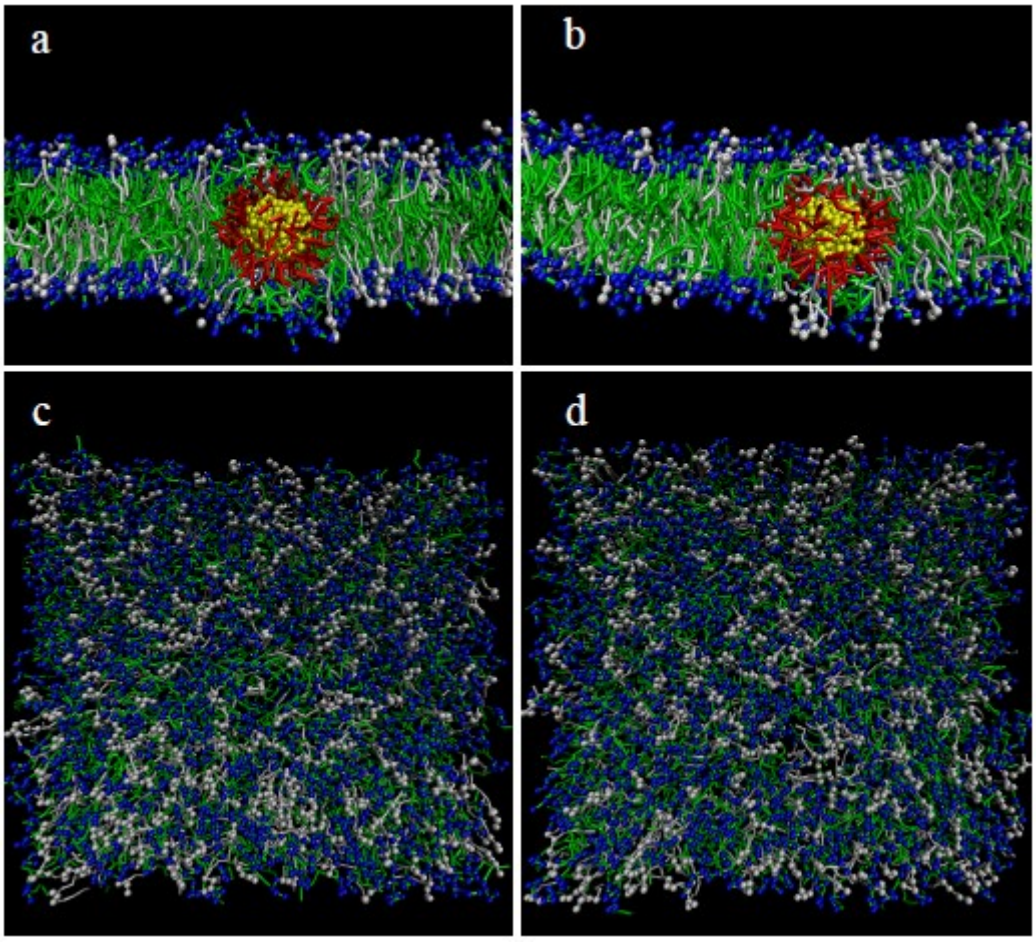

Figure S1. Snapshots of simulations accomplished for nanoparticles with 15% (a and c) and 25% (b and d) of charge. These results are in agreement with nanoparticles with 20% of charge, as noted in the article main text.

2. **Density profiles**

Density profiles for nanoparticles with 40, 60 and 80% of charge are plotted in Figure S2. These results show that the nanoparticle was adsorbed on the membrane surface for all charge densities.

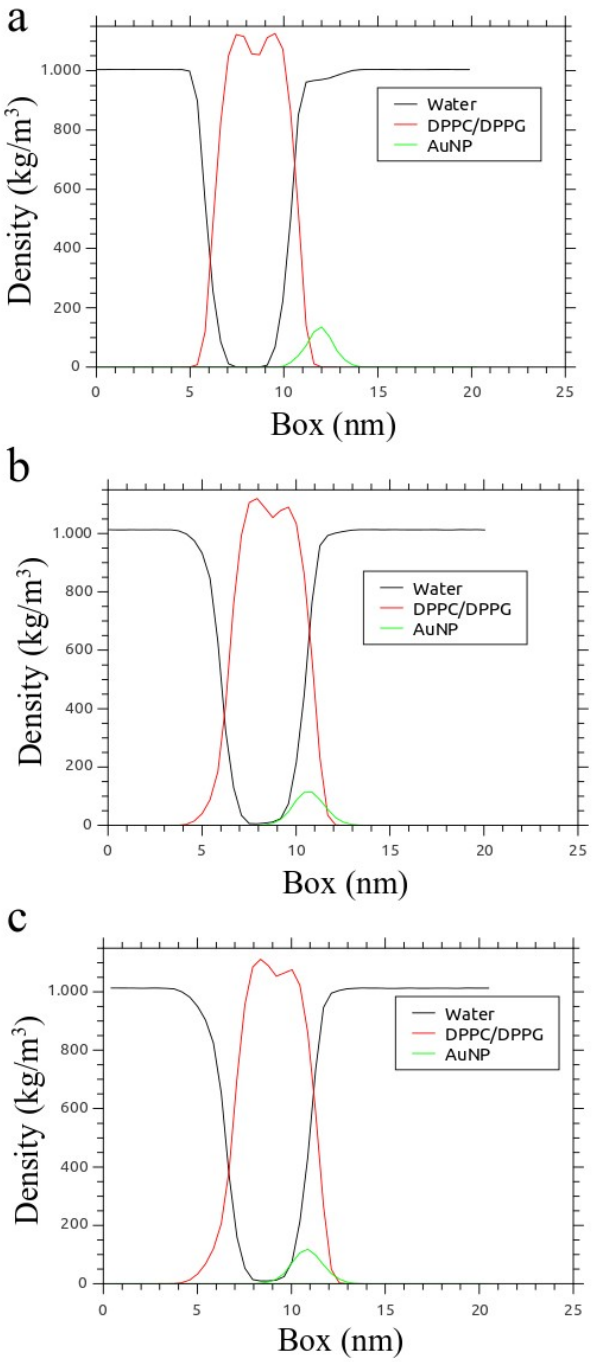

Figure S2. Density profiles after the interaction with nanoparticles with (a) 40% of charge, (b) 60% of charge and (c) 80% of charge

In Figure S3 (a) and (b), density profiles of the DPPC and DPPG lipids, nanoparticle and water are plotted for simulations with 20% and 100% of charge. Insets are snapshots of the trajectories at the end of simulations. Mass density of nanoparticle inside the membrane region Figure S3 (a) indicates that nanoparticle is able to move into the hydrophobic region, although complete translocation was not observed as might be expected in vitro or in vivo. This behavior is not observed in the cases 40, 60 and 80% of charge although density profiles indicated an adsorption of nanoparticle on membrane surface.

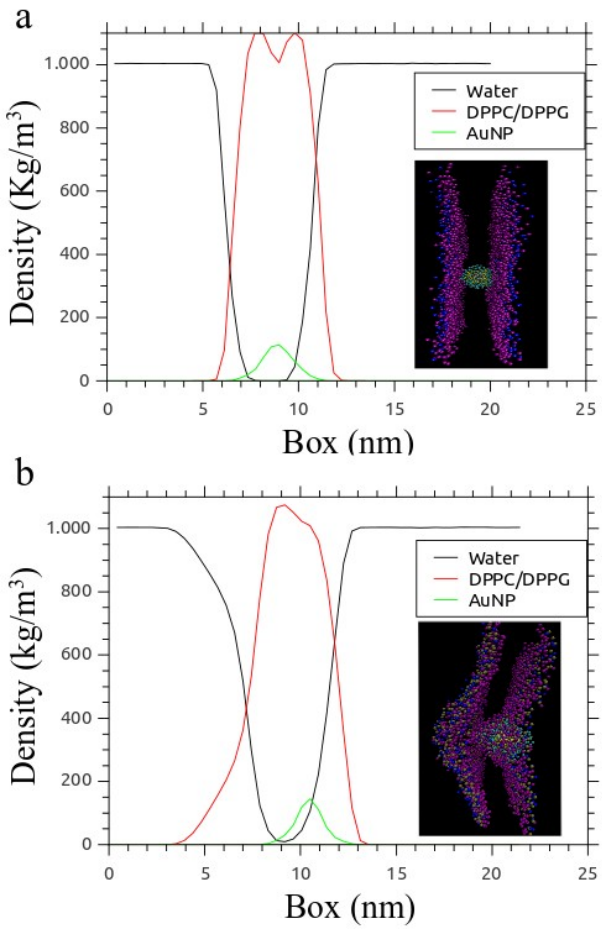

Figure S3. Density profiles after the interaction with nanoparticles with (a) 20 \% and (b) 100% of cationic charge density.

On the other hand, mass density (Figure S3 (b)) indicates that the nanoparticle is inside the bilayer region but in a different way. In this case, instead of a pore formation, nanoparticle is wrapped by the membrane and remains outside the hydrophobic region, as shown by inset in the Figure S3 (b).

3. **Simulations performed with 40×40nm**

Simulations using a 40×40 nm membrane were also performed to evaluate the behavior for nanoparticle interaction compared with 20×20 nm membranes. As can be observed,

these results are in agreement with simulations with 20×20 nm biomembranes. These simulations were 100 ns long.

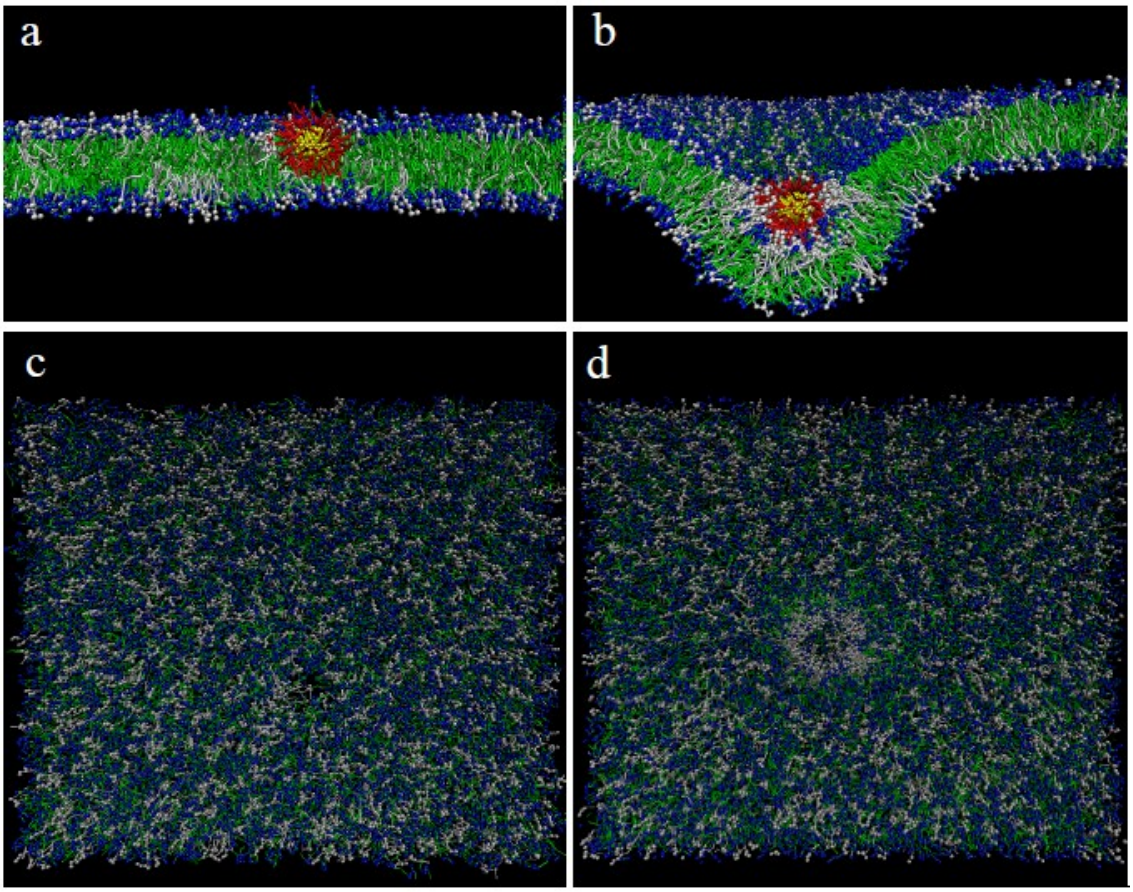

Figure S4. Simulations accomplished using larger membranes (40×40nm). Figure S4 (a) and (c) are snapshots for a nanoparticle with 20\% of charge. Figure S4 (b) and (d) are from simulations using a 100\% of charge nanoparticle.

4. Defective area and shrinkage area

The defective area was calculated using the equation

$$S_d = N.L - S_n$$

where S_d is the defective area, L is the area per lipid of an intact bilayer, N is the number of lipid groups in the disrupted area of the bilayer after interact with nanoparticles and S_n is the corresponding surface area (see Supporting information of the Ref. 23).

The shrinkage area was calculated using the GROMACS tool g_energy, taking the x,y box dimensions and calculating the corresponding area before and after nanoparticle-membrane interactions.