of the L2 bilayer to the L3-embedded NPs is enough to compensate for the elastic deformation of the L2 bilayer, which adapts to the curvature imposed by L3.

As a final test, we designed an *in silico* experiment in order to demonstrate the possibility for an aggregate of semi-snorkeled NPs to induce negative curvature on an interacting liposome. We built a simulation box containing a membrane with a semi-snorkeled NP aggregate, and a bicelle (top snapshot in Figure 5.5b). If isolated, the bicell would close and form a small liposome. However, after a few tens of nanoseconds, the bicelle lays on top of the underlying NP aggregate, developing a local negative curvature, as shown in the picture.

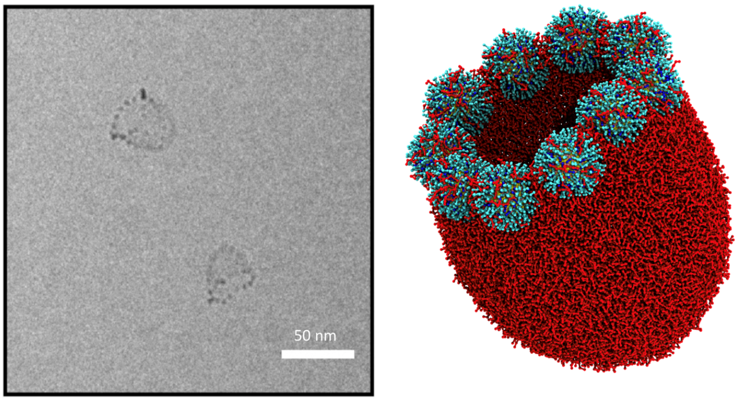

Figure 5.6: **Jellyfish configuration: open liposome** On the left, an experimental image containing unusual liposome structures, in a system of DOPC solvated with MUS:OT 30% OT (2.1 ± 1 nm) NPs. On the right, our interpretaion of these structures: a jellyfish-like structure composed of a small, open liposome sealed by a ring of NPs.

Interestingly, the strong positive curvature induced by semi-snorkeled NPs can also lead to the formation of peculiar structures, as the ones shown in Figure 5.6, left. The experimental image, along with many similar others [61], suggests the presence of open liposomes, in which the edge of the pore is decorated by NPs. While it isn't possible to observe the spontaneous formation of the open liposome configuration in unbiased simulations, we can artificially set up the system. This configuration, with the NPs sealing the pore, remains stable for at least 10 µs, where the same structure without NPs would close in a few tens of nanoseconds. This is an extreme example of stabilization of positive membrane curvature induced by the NPs, since we can interpret the membrane edge as very high curvature region.

5.3 CONCLUSIVE REMARKS

In conclusion, we have shown that aggregates of NPs at different stages in the membrane penetration process are able to impose different curvatures to the bilayer. Aggregates of NPs that are simply adsorbed on the membrane surface induce a slight negative curvature, with a range of deformation which does not exceed one or two NP diameters. The most pronounced effect on membrane curvature is obtained when the NPs are in the semi-snorkeled configuration, i.e.

the process of penetration is in an intermediate stage: in this configuration the aggregate cause the membrane to develop a very rigid positive curvature, over the length of several NP diameters. The length of the anionic NP ligands is a key parameter in this process, because anchoring to the distal leaflet cause it to heavily deform. Another key factor is the slow kinetics of the NP embedding process, which takes longer than the characteristic time of diffusion, allowing NPs to form large aggregates and impose different curvatures to the underlying membrane. When aggregates of NPs semi-snorkeled or adsorbed on a liposome make contact with another liposome, they can originate different interfaces depending on their membrane penetration state. The different curvature that they impose to the bilayer is the key to understand the experimental images which show both flat and curved liposome-liposome interfaces. Aggregates of adsorbed NPs can flatten the liposome membrane, while aggregates of semi-snorkeled NPs well adapt to the positive curvature of the liposome, stabilizing it further. The molecular mechanism observed using molecular level simulations offer an interpretation to the peculiar experimental observations of both flat and curved liposome-liposome interfaces.

6

CONCLUSIONS AND PERSPECTIVES

In this thesis we presented our work on the aggregation of NPs in water and at the biomembrane interface. Our research has been developed using computational methods, in particular the production and analysis of simulations obtained with MD and advanced sampling techniques. The results are important since they shed light on the aggregation behaviour of widely used and studied NPs, and on the effects of this aggregation on the membrane properties. Moreover, our findings offer fundamental insights on the physical properties of soft, nanoscale interfaces, which are transferable to other biologically relevant processes.

Hydrophobic carbon nanoparticles: size dependent membrane aggregation

In Chapter 3 we explored the aggregation behaviour of hydrophobic spherical membrane inclusions with different sizes. The models are developed to represent the surface of fullerenes, and indeed the F16 model, comprised of 16 bead, represents the C_{60} fullerene. The other models are composed of 64, 216 and 576 beads respectively, and their diameter goes from 1 to 5 nm.

We observed that the behaviour of these NPs in the membrane is indeed strongly dependent on their size. The smallest NPs, coherently with experimental observations[80, 81], are almost completely soluble in the hydrophobic environment of the lipid bilayer's core. On the contrary the largest NPs, which diameter is as large as the bilayer thickness, form stable 3D clusters, causing the bilayer to deform significantly. This is a clear effect of the finite size of the membrane bilayer, that behaves as a 2D solvent only for small inclusions.

The intermediate sized NP shows a peculiar behaviour: they form linear, chain-like aggregates inside the membrane. Since the NP shape is isotropic, there isn't a trivial explanation for this aggregate shape. Tuning the curvature of the membrane, we observe that these aggregates are indeed strictly correlated with membrane undulations. Moreover, the presence of the aggregates is able to induce region of pronounced curvature in the membrane, even forming folds of several tens of nanometers. We observed that this behaviour depends on the fact that the NP does not lie at the center of the bilayer, but is slightly displaced toward one of the leaflet, thus inducing a local curvature. This fact explains the ability of these NPs to both sense and induce curvature, as well as the asymmetric shape of its aggregates [211].

The unexpected aggregation of same-charge amphiphilic Au NPs in water and lipid membranes

The investigation on NP-NP aggregation is carried on and developed in Chapter 4, changing the subject to functionalized AuNP, in particular negatively charged amphiphilic NPs. Compared to the spherical NPs of the Chapter 3, these are multicomponent, complex nanomaterials, and their surface is amphiphilic and able to reshape. Thus, their interactions in water are not easy to predict, and indeed their behaviour is peculiar. Experiments and simulations [154] show that, despite having a negatively charged surface, MUS:OT coated NPs are not completely soluble, but form stable clusters of several NPs.

Our simulations prove that aggregation is driven by the interplay of two different NP-NP dimerization configurations. The first is ion-bridging, in which several counter-ions link the negatively charged terminals of the MUS ligands of two NPs. The second is the hydrophobic contact configuration, where the two NP ligand shells interpenetrate and bring the NP cores to almost contact each other. We observed that the propensity to form one bond or the other depends on the size of the NPs core and on the ligand shell hydrophobic content (OT): the higher the surface charge density, the more favourable ion-bridging gets. Moreover, the reshaping of the ligands coating leads to non-pairwise additive interaction. Indeed, the more hydrophobic contact bonds a NP makes, the less favorable it is for it to form another. This leads to anisotropic, composition-dependent aggregate shapes, ranging from 3D clusters of dimers to linear chains or ribbons.

The experimental images show that aggregates of MUS:OT NPs are also found adsorbed and embedded in the DOPC membrane[220, 103]. In this case, the aggregation can be driven by different factors depending on the state of NP penetration in the membrane. While for adsorbed NPs the ion-bridging is still the dominating aggregation agent, when the NPs are semi or fully embedded the membrane became a mediator of NP-NP interaction. The fully snorkeled NPs, which are symmetrically embedded in the bilayer, attract each other due to a lipid depletion that they induce in their surroundings (see Section 1.3.1). Lastly, the semi-snorkeled NPs remind of the F216 NPs of Chapter 4, in which they induce significant, positive local curvature to the bilayer due to their asymmetric embedding. In this case the driving force of aggregation is elastic energy minimization (Figure 1.12d), together with ion-bridging stabilization.

Liposome-liposome aggregation induced and affected by amphiphilic gold NP clusters

The study of NP aggregation carried out in Chapter 4 naturally led to the study of aggregation of larger structures: liposomes. Indeed, the same experimental works that revealed the presence of NP aggregates at the membrane interface also show that the NPs also mediate the interaction between different liposomes [9, 220, 188], which were the model membrane in the experimental setup. In Chapter 5 we studied the liposome-NP-liposome interface, and how it is affected by the aggregation of NPs. This was an interesting problem since the experiments show the ability, for the same liposome, to form radically different interfaces, with membrane flattening or even curvature inversion, without an apparent explaination.

The reason for this process lies in the different states of aggregation of the NPs which in turn derive from the different penetration states, as studied in Chapter 4: aggregates at different penetration stages induce different curvatures to the bilayer. When the aggregate is composed of semi-embedded NPs, the induced curvature is positive and very stable. When the NPs are adsorbed instead, their aggregates induce a slight negative curvature. This explains the different interface shapes. If the NP aggregate is adsorbed on both liposomes, the membrane is flattened symmetrically. If instead one of the aggregates is semi-embedded and the other adsorbed, the interface is asymmetric: the liposome with the semi-snorkeled aggregate will not flatten, and the liposome with the adsorbed aggregate inverts its curvature.

The propensity of semi-embedded NPs to stabilize high curvature regions also explains the observation of peculiar, open liposome configurations observed in the experimental images. The NPs form a ring on the edge of the liposome, stabilizing it and preventing its complete formation.

It is important to note that in Chapter 4 and 5 the use of MD and its related techniques and analyses allowed us to draw an exhaustive picture of the NP-membrane system, for which the experimental data offered a fascinating and detailed but incomplete view, due to the static nature of the employed techniques. Starting from the study of how the NPs aggregate in water, to their aggregation mediated by the membrane, we eventually explored their role in mediating aggregation at another level, that of liposome-liposome interaction. Overall, our results contribute to the fundamental understanding of synthetic NP-membrane interactions, and highlight the importance of the unique physical properties of the soft, deformable NP ligand shell.

Perspectives

Since NPs are already produced and used in biomedicine[35, 22, 115], as therapeutic or diagnostic devices (or both [173]), it is crucial to understand their aggregation behaviour in water. This is especially true for negatively charged NPs, in which the charged terminal ligand's role is that of assuring colloidal stability. Our results show that aggregation is indeed possible despite this specific design, and that the aggregate's shape depends in a non-trivial way on the NP cores size and ligand shell composition. These findings open up a wide design space for new NPs specifically tailored to form aggregates with the desired shape and size, which could be exploited in advanced biomedical applications [72].

The comparison of the results obtained studying different aysmmetric membrane inclusions (hydrophobic or amphiphilic) allowed to generalize our knowledge of the driving forces controlling aggregation in the membrane. This knowledge could be further extended by considering inclusions with a more varied ligand shell, with longer or chemically different ligands. In this perspective, another interesting line of study would be exploring the effects of anisotropy in membrane inclusions. This would allow to mimic the shape of larger, biological membrane inclusions, for instance BAR-domain proteins [153], which are involved in many relevant processes inside and outside the cell. One such process is vesicle-membrane fusion, which is mediated by membrane reshaping proteins.

The results presented in Chapter 5 show that amphiphilic NPs are able to mediate liposome-liposome aggregation, even with significant structural rearrangements of the liposome-liposome interfaces. These configurations resemble the first step of the biological membrane fusion process. Since we never observed the next steps in our simulations, it is apparent that other factors are necessary for the fusion process to progress. Recent experimental research show that the very same amphiphilic NPs, when in combination with Ca^{2+} divalent ions, have the ability to trigger membrane fusion [188]. However, the molecular mechanisms by which these NPs enhance fusion are not well understood yet. To a certain degree, this lack of knowledge about molecular details extends to the case of the biological counterpart of this process, i.e. protein induced fusion [45, 84, 64]. Exploiting the tunability of the ligand shell of these amphiphilic NPs, it is possible to investigate the main structural features that these fusion agents must have in order to efficiently enhance membrane fusion.

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