Mechanism of Vesicle Spreading on Surfaces: Coarse-grained Simulations

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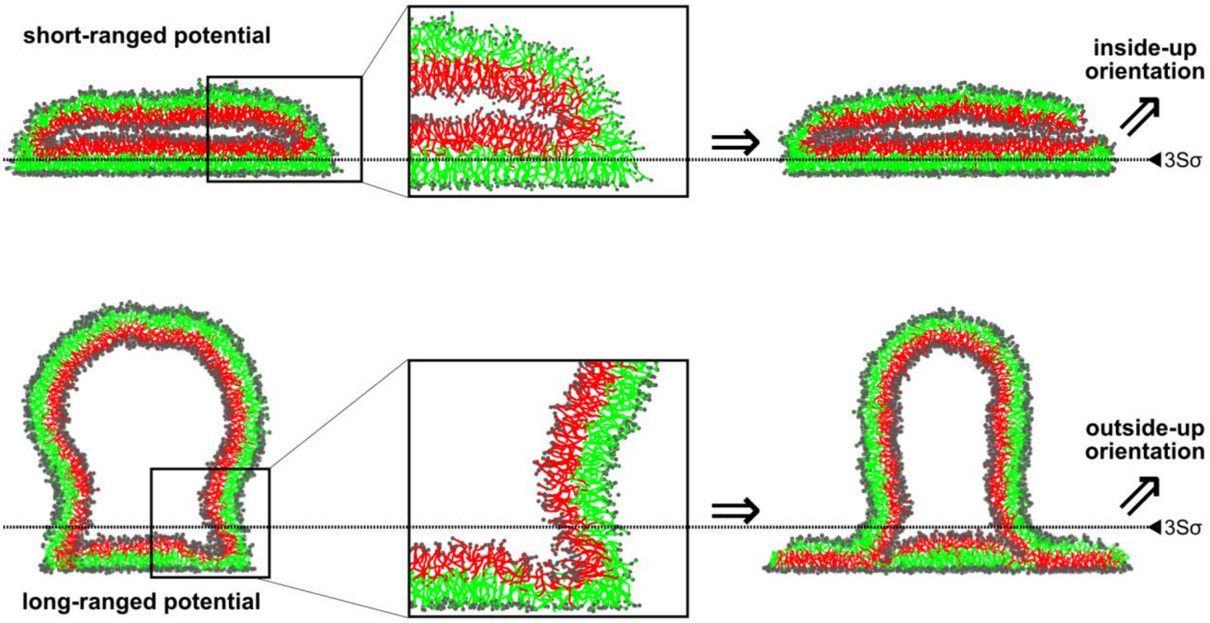
Abstract

Exposition of uni-lamellar vesicles to attractive surfaces is a frequently used way to create supported lipid bilayers. Although this approach is known to produce continuous supported bilayers, the molecular mechanism of their formation and its dependence on factors like surface interactions and roughness or membrane tension as well as the interplay between neighboring vesicles or the involvement of pre-adsorbed bilayer patches are not understood very well.

Using multibody dissipative particle dynamics simulations we assess different mechanisms of vesicle spreading on attractive surfaces, placing special emphasis on the orientation of the resulting bilayer. Making use of the universality of collective phenomena in lipid membranes, we employed a solvent-free coarse-grained model, enabling us to cover the relatively large system sizes and time scales required. Our results indicate that one can control the mechanism of vesicle spreading by tuning the strength and range of the interactions with the substrate as well as the surface's roughness, resulting in a switch from a predominant inside-up to an outside-up orientation of the created supported bilayer.



The simulations provide insights into the molecular mechanisms of spreading, which subtly depend on the lipid conformations at the highly bent rim of the adsorbed vesicle. The figure above schematically represents two distinct spreading pathways that we have observed in our simulations. Longer-ranged interactions between the surface and lipids as well as surface protrusions or roughness tend to prefer the outside-up orientation of the adsorbed bilayer. Additionally, we observe that the spreading of filled vesicles tends to proceed slower than that of leaky or non-filled vesicles and that crowding of vesicles on the surface or pre-adsorbed bilayers speed-up the spreading process.