# Dynamics of Lipid Bilayers Influenced by Truncation of Electrostatic Interactions

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## Introduction

Soft–matter systems such as lipid membranes are often influenced or even governed by electrostatic interactions. Proper treatment of electrostatic interactions in molecular dynamics (MD) simulations of biophysical systems is therefore one of the most important issues in this field, and it continues to pose significant challenges for computer simulations.

In this work, we provide compelling evidence that different treatments of electrostatic interactions in MD simulations may dramatically affect both structural and dynamic properties of lipid membranes.

## Model of DPPC bilayer

- DPPC (dipalmitoyl phosphatidylcholine) bilayer composed of 128 DPPC molecules fully hydrated by 3655 water molecules (SPC).
- United atom GROMACS force field
- $T = 323$ K, time scale 50 ns
- A full description of the system is given in Refs. [1,2].
- Electrostatics: Particle-Mesh Ewald (PME) or truncation at 1.8 – 2.5 nm

## Results

Results for the area per lipid molecule shown in Fig. 1 illustrate that truncation leads to compressed bilayers with respect to the PME case. The PME results are consistent with experiments [3], i.e. $\langle A \rangle \approx 0.64\,\mathrm{nm}^2$.

Consequently, as demonstrated in Fig. 2, truncation enhances the ordering of acyl chains.

Figure 3 illustrates how the dynamic properties of the system are influenced by truncation. We find that the lateral diffusion coefficient is $(12.7 \pm 0.5) \times 10^{-8}\,\mathrm{cm}^2/\mathrm{s}$ using PME, in agreement with experiments [4], while the truncation at 1.8 nm gives $(1.3 \pm 0.3) \times 10^{-8}\,\mathrm{cm}^2/\mathrm{s}$. That is, the truncation slows diffusion down by a factor of ten. Rotational diffusion is affected accordingly (Fig. 4).

Where do these subtle differences come from? Figure 5 shows data for radial distribution functions for N–N pairs in the DPPC headgroups. While the PME result is consistent with the fluid-like phase ($L_\alpha$), the truncation gives rise to artificial peaks precisely at the truncation distance.

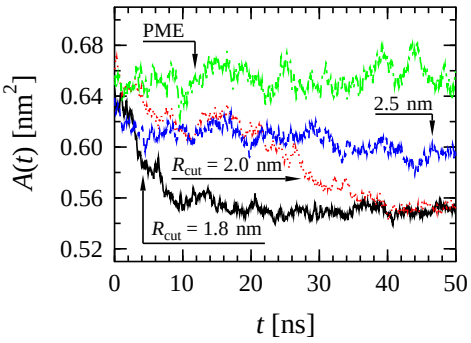


Fig. 1: Evolution of the area per molecule in time.

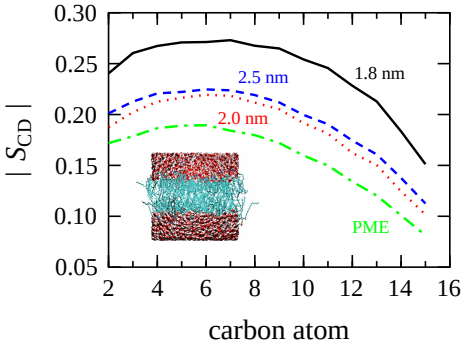


Fig. 2: The order parameter $S_{CD}$ for the *sn-2* chain of DPPC molecules.

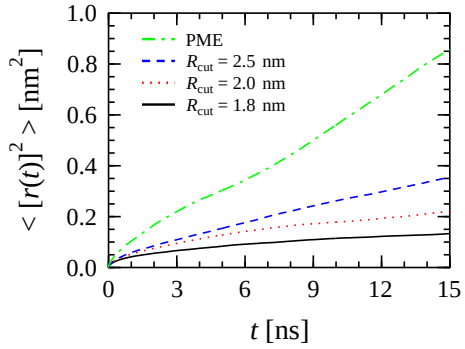


Fig. 3: Results for the mean-square displacement in time: lateral diffusion of DPPC molecules.

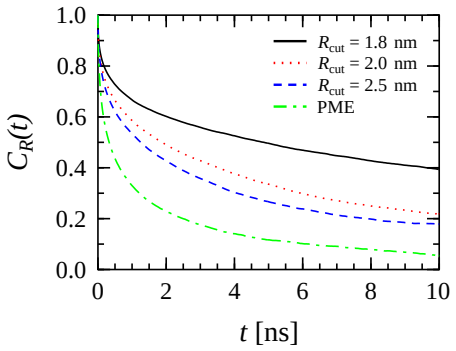


Fig. 4: The correlation function of rotational diffusion along the P – N vector in the headgroup of DPPC.

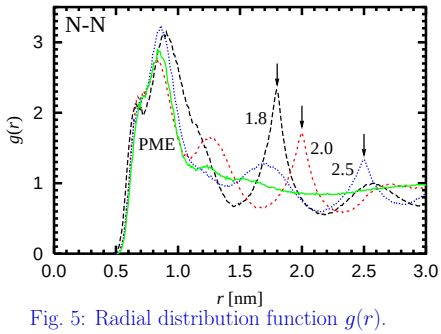


Fig. 5: Radial distribution function $g(r)$.

## Conclusions

Truncation of electrostatic interactions can lead to serious artifacts in lipid membrane systems. In particular, it may give rise to artificial peaks in pair correlation functions, and thus change the phase behavior of the system. We conclude that truncation is not the method of choice for incorporating electrostatic interactions into model systems of lipid membranes.

It is expected that the same conclusions apply to many other biologically relevant soft-matter systems where electrostatics play a crucial role, such as DNA-lipid complexes and proteins in membranes. Particular care is therefore called for in all these cases.

### References

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