A Coarse-Grained model for peroxidized lipid membranes

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Lipid oxidation is a natural phenomenon occurring in living cells, which may result in significant alterations of the biological membrane properties. Oxidation is also a side effect (intentional or not) of using fluorescent dyes for biomembrane imaging. Dye sensitized singlet oxygen production, in particular, converts insaturated lipids into peroxidized molecules.

Recent works [1,2] demonstrated that lipid peroxides can be generated in a controlled manner, leading for the first time to the determination of physical and structural properties of peroxidized bilayers.

We present here an original model for coarse-grained peroxidized lipid membrane simulations, and compare our findings with the experimental available data of ref. [1,2]. Our approach provides new insight on the lipid reorganisation following peroxidation [3]. The normal-oxidized lipid mixing properties will also be briefly discussed.

[1] Weber et al., Soft Matter 10, p4241 (2014)

[2] P. H. B. Aoki et al. , DOI: 10.1039/C5SM01019E, Soft Matter (2015)

[3], Y. Gua, V.A. Baulin, F. Thalmann, submitted.