3rd URSI AT-AP-RASC, Gran Canaria, 29 May – 3 June 2022

Hydrated lipid bilayers and RF EM fields: an insight through Molecular Dynamics simulations

Laura Caramazza*(1), (2), Paolo Marracino (3), Micaela Liberti (1), (2), Francesca Apollonio (1), (2)

(1) Department of Information Engineering, Electronics and Telecommunications, Sapienza University of Rome, Italy; e-mail: laura.caramazza@uniroma1.it; francesca.apollonio@uniroma1.it; micaela.liberti@uniroma1.it
(2) CLN2S@Sapienza, Fondazione Istituto Italiano di Tecnologia, Rome, Italy;
(3) Rise Technology S.r.l., L.re Paolo Toscanelli 170, Rome, Italy; e-mail: paolo.marracino@risetechnology.com

Molecular simulations aim to compute macroscopic behavior from microscopic interactions; in particular, Molecular Dynamics (MD) techniques investigate the conformational rearrangements of molecules and their interactions with other molecular species and with external applied physical stimuli as electromagnetic (EM) fields. The main strength of MD simulations is the amount of detail which makes possible to take into account all or nearly all atoms incorporated into the model at the cost of huge computational power [1]. MD simulations provide thus a powerful, complementary approach to experiments, such that they have been used to extensively study many biological targets as proteins, enzymes and particularly lipid bilayers [2]. These last ones, acting as selective barriers for the permeation of molecules, and playing key roles in modulating the dynamics, organization, and function of membrane proteins, can be recognized as the preferential target of EM fields.
Models of hydrated lipid bilayers have been already investigated in literature, when coupled with electric field pulses of extremely short duration (ns) for the comprehension of the mechanism of pore formation [3, 4] at the basis of medical electroporation purposes. However, the response of a lipid bilayer to a radiofrequency (RF) EM field has been less studied [5], despite its importance for the physical insight of the interaction between membranes and EM fields.
In the present work, MD simulations of a hydrated lipid bilayer embedded in a conductive ionic solution (Figure 1) are studied in presence of an external EM field of 1 GHz frequency. Results are reported in terms of dipolar coupling of both water and lipids with the applied RF field, comparing outcomes with a static field and with homologous models where no ions have been included. The MD simulations were performed using the GROMACS software version 4.6.5. The hydrated bilayer system was constructed starting from 512 POPC lipid molecules and more than 53000 Simple Point Charge (SPC) water molecules.

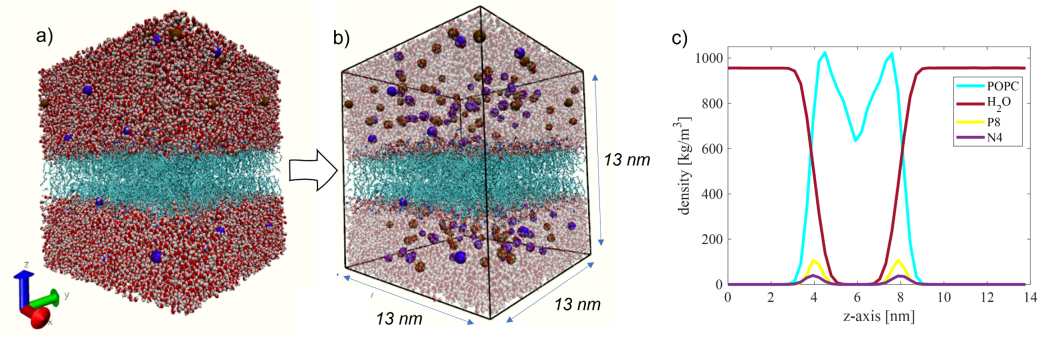

Figure 1. a) 3D model used for MD simulations where water molecules (red and white), lipids (cyan acyl chains and red headgroup), ions (K^+ and Cl^-, violet and ochre spheres, not in scale) are reported. b) 3D details of the internal structure (water in transparency) and initial dimension of the model. c) Density distribution profiles along the z-axis of POPC and water molecules, together with P8 and N4 atoms of the lipid heads without the external field.

References

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