Plasma-induced oxidation of the lipid bilayer: Insights from molecular level modeling

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Near room temperature or cold atmospheric plasmas (CAPs) are gaining increasing interest for cancer treatment [1-3]. The underlying mechanisms, however, are still not fully understood, but they are important in terms of safe utilization. It is largely accepted that CAP-generated reactive oxygen and nitrogen species (RONS) play a key role [3-5]. Indeed, a noticeable rise of intracellular ROS has been observed in cancer cells compared to normal cells upon CAP treatment [6-9], which can eventually result in oxidative damage inside the cells. The CAP-generated species first interact with the cell membrane, thereby oxidizing its lipids, and it is important to study the behavior of the oxidized membrane and its effect on the penetration abilities of the RONS across the oxidized lipid bilayer.

This talk will give an overview of our recent simulation results on the interaction of ROS with the lipid bilayer which causes lipid oxidation, thereby leading to increased membrane fluidity. Moreover, insights on the permeation of various (hydrophilic and hydrophobic) RONS through both oxidized and non-oxidized membranes will be provided, and the synergistic effect of the electric field and lipid oxidation, both arising from CAP, on the permeability of cell membranes, will be explained, as well as the phosphatidylserine (PS) flip-flop induced by lipid oxidation, which plays a vital role in apoptosis signaling. Finally, the results on the different permeability of H_2O_2 across aquaporin transmembrane channel vs. the lipid bilayer will also be demonstrated.

References

[1] Keidar M., *Plasma Sources Sci. Technol.* **24** 033001 (2015)
[2] Keidar M. *et al.*, *Br. J. Cancer* **105** 1295 (2011)
[3] Ratovitski E. A. *et al.*, *Plasma Process. Polym.* **11** 1128 (2014)
[4] Graves D. B., *Plasma Process. Polym.* **11** 1120 (2014)
[5] Lu X. *et al.*, *Phys. Rep.* **630** 1 (2016)
[6] Kim S. J. *et al.*, *Appl. Phys. Lett.* **103** 153705 (2013)
[7] Ishaq M. *et al.*, *BBA Mol. Cell Res.* **1843** 2827 (2014)
[8] Ishaq M. *et al.*, *Mol. Biol. Cell* **25** 1523 (2014)
[9] Kaushik N. K. *et al.*, *PLoS One* **9** e103349 (2014)