Ions, membranes and channels: from the quantum level to continuum modelling

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The application of short and intense electric pulses enables to transiently alter the properties of cell membranes, making them permeable to a wide range of chemical species. This phenomenon is routinely used in medical applications as well in biotechnology and industrial processing. Most investigations to date of the processes involved have focused on the ability of intense electric fields to create pores within the lipid bilayers, allowing us to better understand and control the phenomenon termed "electroporation". Our knowledge on the other hand, about the chemical processes enhanced as a consequence of the application of electric fields to cells is still sketchy. In this contribution we harness the capabilities of computational resources and the predictive power of advanced atomistic and quantum level molecular dynamics techniques to decipher key steps in several chemical and biophysical processes occurring during and following Electric field stimulations of cell membranes. We show that under low-voltage conditions, and predict that under sub-nanosecond pulse electroporation conditions, peroxidation of model cell membranes by potent reactive oxygen species (OH• and OOH•) is significantly enhanced. We quantify the permeability of the peroxidized membranes to a host of species including ions and molecules, to demonstrate that electrically mediated chemical effects may play a significant role in several processes following exposure of cells to high electric fields. We discuss the relevance of these effects for cells subject to radio-frequency electromagnetic fields (RF-EMF) as well as for excitable cells subject to electro-stimulation.