Molecular dynamics simulations of the permeation characteristics of plasma active species into biological membranes

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Recently, plasma medicine has been rapidly developing as a new research field with the technical establishment of the formation of cold atmospheric pressure plasma (CAP). The medical effects are strongly related to the radicals and ions generated by the CAP. These species penetrate cell membranes and react with intracellular substances. However, the detailed mechanisms of biological interactions are not well understood because of the complicated physicochemical processes in living cells. In this study, we simulated the spatio-temporal behavior of reactive oxygen and nitrogen species (RONS) in a biological membrane using molecular dynamics. Some permeation properties of RONS against the membrane, especially under electric field, were also discussed.