سمینار هفتگی ماده چگال نرم

# Article Review: "Reactive and non-reactive molecular dynamics simulations of plasma-biomolecule Interactions for a better insight into plasma medicine"


## Abstract

"Cold Atmospheric Plasma (CAP) is an ionized gas consisting of free radicals, ions, electrons, reactive neutral species, photons and electric fields which recently has many biological applications including cancer treatment, wound healing, microorganisms (i.e., bacteria, fungi, and viruses) inactivation, skin disease treatment, and blood coagulation. Among all products of CAP, reactive oxygen and nitrogen species (RONS) play the most important role in medical treatment. During CAP treatment, cell membranes, and membrane proteins are the first cellular components that can be chemically modified by RONS. Structural changes of RONS-modified membrane can disturb the normal permeability of the membrane to different substances such as RONS produced by CAP. Increasing the rate of RONS entry into the cell makes an imbalance between the intracellular RONS level and antioxidant system leading to oxidative stress that can damage proteins, lipids and DNA which are effective in protein-protein, protein-lipid, and DNA-protein interactions and disturbs the normal function of the cell organelles. The membrane also maintains the membrane proteins on or inside itself which have different functions for the cell and can be structurally changed by RONS and lose their normal functions. To better understand the details of the interactions between RONS and cellular components, which are beyond the scope of experimental techniques, computational simulations can be beneficial. Among all computational simulations, reactive and non-reactive molecular dynamics (MD) simulations are a very powerful method that can be used to investigate the evolution of biological systems, considering their size and time scale. By using MD simulation, biological conditions close to reality can be designed and investigated. To study the evolution of a large system and investigate the interactions between macromolecules non-reactive MD simulation is an appropriate method. This presentation discusses the applications of non-reactive MD simulations in bio-plasma to provide a better overview of CAP in medicine."



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