Molecular Dynamics: A Valuable Tool in Plasma Medicine – Dr. Cecilia Oliveira

Plasma medicine is an emerging field with applications in skin disease treatment, tooth bleaching, blood coagulation, sterilization, wound healing, and cancer therapy. Despite its success, the underlying mechanisms of plasma interactions with biological systems remain poorly understood. Molecular dynamics (MD) simulations offer a powerful complement to experiments, enabling atomic-level investigation of interactions that are often inaccessible experimentally.

MD simulations have been instrumental in studying plasma-generated reactive oxygen and nitrogen species (RONS) and their interactions with biomolecules such as proteins, lipids, DNA, and RNA. These studies reveal that RONS can induce structural and conformational changes in biomolecules, compromising cell function and contributing to bacterial disinfection, wound healing, and cancer cell death. For example, oxidation of membrane lipids and proteins can lead to pore formation and membrane rupture, ultimately causing cell death.

MD also helps elucidate the effects of electric fields and plasma-derived ions, offering insights into optimizing plasma treatments. Key challenges remain, including defining realistic model systems that are both computationally manageable and biologically relevant, and ensuring force-field accuracy. Despite these limitations, MD provides a valuable framework for understanding plasma-biomolecule interactions and guiding the development of more effective plasma-based therapies.

Curriculum vitae of Dr. Cecilia Oliveira

Cecilia Oliveira obtained a PhD in Chemistry in 2022 from the Federal University of ABC, Brazil, and the University of Antwerp, Belgium. Since her master's program, her research has focused on molecular simulations of biological systems, including membranes and proteins, under oxidative conditions to improve anticancer therapies based on oxidative stress.

She employs molecular dynamics simulations and quantum calculations to characterize biological systems at the atomic and molecular level. Since 2023, she has been a postdoctoral researcher at the University of Antwerp, combining computational and experimental approaches to study the use of plasma in cancer treatment. Future research plans include simulating more complex systems, such as hydrogels and carbon nanotubes, to further enhance the effectiveness of plasma-based therapies.