# Molecular dynamics simulation of plasma-bacteria cell wall interaction

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Low-temperature, non-thermal atmospheric plasmas have important applications in medical fields, including sterilization of surfaces and diagnostic devices, as well as for therapeutic techniques, e.g. wound healing and treatment of cancer and skin diseases. As a result, there is currently an increasing interest in plasmas for medical applications.

However, modeling of both the plasma itself and the interaction of plasma with living organisms such as bacteria is very limited until now [1]. Nevertheless, plasma simulations can be useful to obtain information about the density distribution of charged particles, molecules and radicals, their reaction rates, etc., which is difficult to obtain experimentally due to possible plasma disturbance with the measuring tool.

Simulating the interaction of the plasma with the surface of living organisms (e.g. grampositive or gram-negative bacteria) is also very difficult. If a proper interatomic potential can be constructed for describing all relevant interatomic interactions, molecular dynamics simulations can provide atomic scale insight in these interactions.

In the present work, we investigate the interaction of plasma species such as OH, NO, NO2, H2O2, O3 and O atoms with bacterial peptidoglycan (PG) by means of molecular dynamics (MD) simulations. In an MD simulation, the trajectory of all atoms in the system is followed by integrating the equations of motion. Forces on the atoms are derived from the Reactive Force Field (ReaxFF) potential [2]. In this work, we assume the gram-positive bacterium *Staphylococcus aureus* murein as the PG structure, which is typically 20-30 nm thick [3] and serves as a protective barrier in bacteria. Its chemical structure can be found in [4, 5]. Our results demonstrate that among the above mentioned species, only OH radicals and especially O atoms break C-C and C-N bonds, which subsequently leads to a destruction of the bacterial cell wall. This study is important for understanding the chemical damaging of the bacterial PG on the atomic scale.

## References

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