8th Asia-Pacific Conference on Plasma Physics, 3-8 Nov, 2024 at Malacca

# Understanding the mechanisms of cold plasma-induced degradation of antibiotics in hospital wastewater

Maksudbek Yusupov[1], Otamurot Rajabov[1] and Pankaj Attri[2]
[1] Arifov Institute of Ion-Plasma and Laser Technologies, AS Uz
[2] Center of Plasma Nano-interface Engineering, Kyushu University
e-mail (speaker): maksudbek.yusupov@outlook.com

In the field of plasma medicine, cold atmospheric plasma (CAP) is utilized in a range of applications, including sterilization, disinfection, wound healing, dentistry and cancer therapy.[1] In recent years, CAP has been applied to wastewater treatment, showing promising potential in significantly reducing antibiotic effectiveness and achieving successful degradation.[2] Despite extensive research in this area, the basic mechanisms underlying the interaction between CAP and antibiotics remain unclear. Therefore, the objective of this study is to investigate the impact of reactive oxygen species (ROS) generated by CAP on antibiotics using computer simulations. In particular, we employ reactive molecular dynamics simulations based on the density functional-tight binding potential to explore the interaction between oxygen atoms (the main component of ROS) and amoxicillin and/or ofloxacin antibiotics, which are used as model systems in our simulations (Fig. 1).

The simulation results showed that the interaction of oxygen atoms with antibiotics leads to the destruction of the benzene and β-lactam rings in amoxicillin, as well as chemical modifications to the piperazine ring of ofloxacin. Additionally, this interaction results in the creation of $CO_2$ and $H_2O$ molecules along with alcohol and ketone functional groups within the structures, as well as the demethylation of ofloxacin.

This study offers intricate atomic-level insights into the degradation of antibiotics induced by cold plasma, with potential implications for pharmaceutical wastewater treatment applications.

References

[1] M. Laroussi *et al.*, IEEE Trans. Radiat. Plasma Med. Sci., **6(2)**, 127 (2022)
[2] E. Wielogorska *et al.*, Antibiotics, **12**, 1115 (2023)

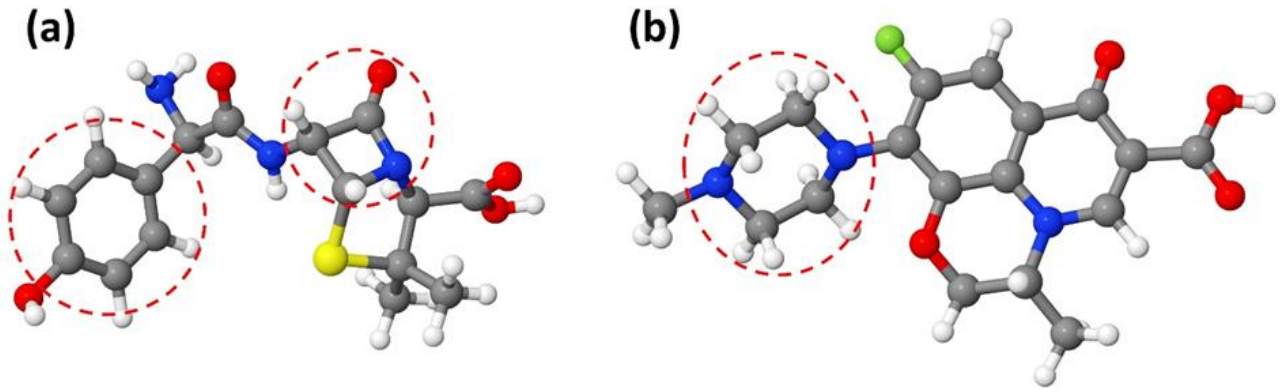


**Figure 1.** Schematic representation of amoxicillin (a) and ofloxacin (b) molecules. In (a), the benzene (left) and β-lactam (right) rings, and in (b), the piperazine ring are indicated by red dashed circles. Carbon, oxygen, nitrogen, hydrogen, sulfur and fluorine atoms are shown in gray, red, blue, white, yellow and green, respectively.