9th Asia-Pacific Conference on Plasma Physics, 21-26 Sep, 2025 at Fukuoka

Atomistic modeling of cold atmospheric plasma effects on antibiotic removal from wastewater: A case study with amoxicillin

Otamurot Rajabov[1], Pankaj Attri[2] and Maksudbek Yusupov[3]
[1] Arifov Institute of Ion-Plasma and Laser Technologies, AS Uz
[2] Center of Plasma Nano-interface Engineering, Kyushu University
[3] Institute of Fundamental and Applied Research, National Research University TIIAME
e-mail (speaker): otamurot.rajabov@outlook.com

Cold atmospheric plasma (CAP) has emerged as a promising technology for wastewater treatment, particularly effective in degrading antibiotics, which are critical contaminants frequently detected in pharmaceutical wastewater [1]. Despite numerous experimental studies, detailed atomic-scale mechanisms behind CAP-induced antibiotic degradation remain unclear, restricting broader adoption and optimization of this technology. This study addresses these gaps by investigating the molecular-level degradation mechanisms of amoxicillin (Figure 1), a widely used β-lactam antibiotic, through CAP treatment using reactive molecular dynamics (MD) simulations.

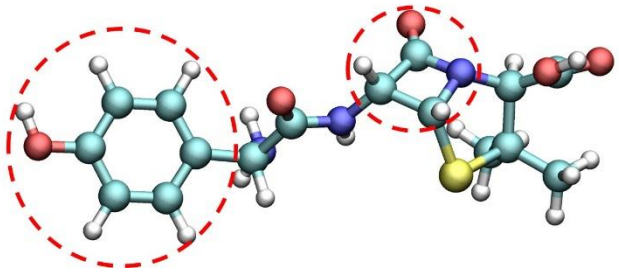

Figure 1. Schematic representation of the amoxicillin molecule. The benzene ring (left) and β-lactam ring (right) are highlighted with red dashed circles. Carbon, oxygen, nitrogen, hydrogen, and sulfur atoms are shown in bluish, red, blue, white, and yellow, respectively.

Simulations based on the density functional tight-binding (DFTB) method were performed to study interactions between reactive oxygen and nitrogen species (RONS) generated by CAP and the amoxicillin molecule. Our DFTB-MD results revealed that some RONS exhibited weak attractive or repulsive interactions, while atomic oxygen (O) and hydroxyl radicals (OH) showed significant reactivity. Specifically, O and OH radicals primarily initiated hydrogen abstraction, leading to substantial chemical modifications, such as the formation of hydroxyl and hydroperoxide groups, opening or cleavage of the β-lactam ring, benzene ring shortening or widening, structural fragmentation, and liberation of small molecules including water, CO_2, and CO. The observed atomic-scale degradation pathways, particularly β-lactam ring opening and hydroxylation, are in excellent agreement with previously reported experimental studies [2-5].

This atomic-scale mechanistic insight substantially enhances our understanding of antibiotic degradation processes induced by CAP, highlighting the pivotal role of O atoms and OH radicals in achieving efficient degradation [6,7]. These findings are fundamental for optimizing plasma-based treatments, supporting the development of more effective, sustainable, and cost-efficient methods for removing antibiotics from pharmaceutical wastewater.

References

[1] C. Sarangapani *et al.*, Sci. Rep., 2019, 9, 3955
[2] W. Li *et al.*, Chemosphere, 2022, 291, 132867
[3] M. Magureanu *et al.*, Water Res., 2011, 45, 3407
[4] D. Klauson *et al.*, Catal. Today 2010, 151, 39
[5] G. Trovó *et al.*, Water Res., 2011, 45, 1394
[6] J. Benedikt *et al.*, Phys. Chem. Chem. Phys., 2018, 20, 12037
[7] M. Yusupov *et al.*, Plasma Process. Polym., 2023, 20, e2200137