Seminar

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Institute for Plasma Research

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Title: Reactive Molecular Dynamics simulation of the carbendazim degradation induced by reactive oxygen plasma species

Speaker: Dr. Ruchi Mishra
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Date: 21st May, 2024 (Tuesday)

Time: 3.00 PM

Venue: Committee Room 4, IPR

Abstract:

In contemporary agriculture, pesticides are extensively utilized to boost the productivity, leaving residues in water, soil, and food items. These residues pose health hazards as they accumulate in organisms, prompting concerns regarding food safety. Carbendazim (CBZ), a systemic benzimidazole carbamate fungicide, used in agriculture, forestry, and veterinary practices to combat fungal diseases, is notably classified as a hazardous chemical by the World Health Organization. Cold Atmospheric Plasmas (CAPs) have demonstrated successful pesticide degradation with notable removal rates, energy efficiency, and eco-friendly attributes. Limited by experimental parameters and equipment availability, scientists are hypothesizing about reaction pathways, which remain elusive. However, through Reactive Molecular Dynamics (RMD) simulations, researchers can now predict breaking and formation of chemical bonds that occur during interactions.

In the present work, we employed RMD simulations to investigate how reactive oxygen species (ROS) induce degradation pathways in CBZ. Our simulations demonstrate that ROS, including O atoms, OH radicals, and O_3 molecules, play a pivotal role in initiating modifications. Typically, the interaction between ROS and pesticides begins with H-abstraction, resulting in the disruption and formation of crucial chemical bonds such as C=C, C-N, and C-O bonds, while facilitating the formation of C-C, C-O, and C=O bonds. Moreover, we examined the dose-dependent effects of ROS on CBZ by incrementally increasing ROS quantities within the simulation environment. As ROS concentration increases, the degree of pesticide damage also increases. The elucidated chemical pathways and statistical data provide insights into the atomic-scale degradation mechanism of CBZ, offering a theoretical foundation for optimizing pesticide degradation strategies in future applications.