

Studying the Effects of Plastics on Proteins and Biomembranes Using MD Simulations and Addressing Environmental Plastic Pollution with AI/ML Methods

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Abstract. *Studying the Effects of Plastics on Proteins and Biomembranes Using MD Simulations and Addressing Environmental Plastic Pollution with AI/ML Methods.*

Plastic particles, especially microplastics and nanoplastics, have become a widespread environmental concern. Originating mainly from the degradation of synthetic materials, these particles are now commonly found in water, soil, and even within biological organisms. Emerging studies suggest that they may interfere with biological systems by interacting with key cellular components such as proteins and biomembranes [ii].

This project combines two complementary research approaches to better understand and address the risks posed by plastic pollution. The first involves classical molecular dynamics (MD) simulations to study how plastic particles affect biological molecules at the atomic scale. Using powerful simulation tools such as LAMMPS and NAMD, we model the interactions between plastic fragments and biomolecules to assess potential structural disruptions, binding affinities, and changes in membrane stability. These insights help to clarify the molecular mechanisms behind observed toxic effects.

The second part of the project focuses on developing and applying artificial intelligence (AI) and machine learning (ML) methods to analyze environmental data related to plastics. By leveraging large datasets, we aim to identify patterns and correlations that may not be visible through traditional analysis. ML models can support the prediction of ecological risk factors, classify plastic particle types, and guide effective strategies for environmental monitoring and mitigation [iii].

By integrating atomistic simulations with data-driven approaches, this project provides a comprehensive framework to study the impact of plastics on living systems and to support the development of solutions for reducing their harmful effects in the environment.

Keywords: Machine Learning, Nanoplastic, Molecular Dynamics