

Showcasing research from Professor Boran Ma's laboratory, School of Polymer Science and Engineering, University of Southern Mississippi, Hattiesburg, MS, USA.

PFAS self-assembly and adsorption dynamics on graphene: molecular insights into chemical and environmental influences

This study employs atomistic molecular dynamics simulations to achieve molecular level insights into PFAS self-assembly and adsorption dynamics to inform PFAS water remediation. Simulation results elucidate the impacts of headgroup chemistry, chain length, and pH on PFAS adsorption efficiency and stability. The findings in this work underscore the complex interplay between PFAS structure and the dynamics of their adsorption behavior, providing guidance for improved PFAS water remediation.

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