

Molecular Insights into Mephedrone Adsorption on Graphene-Based Nanomaterials: A Multiscale Monte Carlo | MD | DFT Study

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The increasing occurrence of new psychoactive substances (NPS) in aquatic environments has raised significant environmental and public health concerns. Among these compounds, mephedrone (4-methylmethcathinone, 4-MMC) is a synthetic stimulant frequently detected in wastewater systems due to its widespread recreational use and incomplete removal in conventional treatment plants [1]. In this work, the adsorption behaviour of mephedrone on graphene (G) and graphene oxide (GO) surfaces was investigated using a multiscale computational approach combining Monte Carlo (MC) sampling, Molecular Dynamics (MD) simulations, and Density Functional Theory (DFT) calculations [2]. Initial adsorption geometries were generated through configurational MC sampling and subsequently equilibrated using MD simulations to account for thermal structural relaxation under near-ambient conditions. The optimized complexes were further refined at the DFT level to determine adsorption energies and electronic properties of the drug–surface interactions. Quantum Theory of Atoms in Molecules (QTAIM), Mayer Bond Order (MBO), and Non-Covalent Interaction (NCI) analyses were employed to characterize the nature of intermolecular interactions. The results reveal that adsorption is dominated by π – π stacking and dispersive interactions on graphene, while additional hydrogen bonding and electrostatic contributions significantly enhance adsorption on graphene oxide due to the presence of oxygen-containing functional groups. The results highlight the potential of graphene-based nanomaterials as promising adsorbents for the removal of emerging psychoactive contaminants from aqueous environments and provide molecular-level insight for the design of advanced nanomaterials for environmental remediation.

References

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Figures

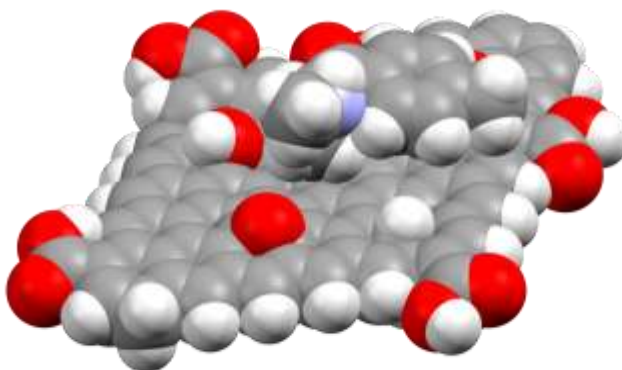


Figure 1: 4-MMC adsorbed onto a graphene oxide sheet.

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