PHOSPHORENE: A NOVEL NANOMATERIAL FOR LIGHT ANTIMICROBIAL THERAPY

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Nanomaterials have attracted significant interest in medical applications due to their high surface area relative to volume, enabling substantial therapeutic loads. Phosphorene has emerged among these materials for its unique properties, including a large surface area, adjustable band gap, and high charge mobility [1]. These characteristics makes phosphorene nanoparticles (BP) particularly promising for photothermal and photodynamic antibacterial treatments through their broad-spectrum light absorption and singlet oxygen production [2-3]. The photoactivity of BP can be amplified by modifying its structure through conjugation with other photosensitizers (e.g. curcumin). [2-3]
This study employs a multi-level computational approach (ab initio quantum mechanics, classical molecular dynamics and Brownian dynamics) to investigate the interaction between BP surfaces and bacterial/viral biomolecules. The West Nile virus (WNV), specifically domain III of the E-protein, was chosen as a model for studying interactions with phosphorene and graphite surfaces.
Initial docking studies, performed using SDA 7.3.3, identified various adsorption orientations of the protein on both surfaces [4]. The most stable and populated structures were then subjected to a series of parallel atomistic MD simulations in explicit solvent, using different initial seeds, to enhance the sampling and assess their stability and folding.
Further analyses revealed differences in the main contact residues and protein stability between the two surfaces, attributed to their distinct chemical natures. Additionally, the interaction of the photosensitizer curcumin with phosphorene was examined. DFT calculations and Xsorb software analyses indicated that curcumin, which is insoluble in water, binds favorably to phosphorene [5]. Subsequent MD simulations incorporated the WNV E-protein into the curcumin-phosphorene complex, providing deeper insight into the system's dynamics.

Key words: phosphorene, PDT, curcumin, antibacterial treatment

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