Advanced Theoretical Investigations into Xylazine Adsorption on Carbon Nanostructures

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The aim of this study is to investigate the adsorption capacities of various carbon nanomaterials for the purpose of Xylazine remediation by integrating sophisticated theoretical methodologies [1]. By leveraging the high surface area and unique properties of carbon nanocones [2], C60 fullerene, graphene, graphene oxide [2], Single-Walled Carbon Nanotubes (SWCNT), and capped SWCNT, we aim to investigate their efficiency in adsorbing Xylazine [N-(2,6-Dimethylphenyl)-5,6-dihydro-4H-1,3-thiazin-2-amine], a veterinary tranquilizer increasingly found as an adulterant in street drugs.

We demonstrate that these nanomaterials have a considerable adsorption potential across the board by using calculations based on the Density Functional Theory (DFT), Molecular Dynamics (MD), and Monte Carlo (MC) simulations [4]. Capped SWCNT has the highest affinity (-106.45 kcal/mol), whereas C60 fullerene demonstrates the lowest affinity (-51.92 kcal/mol). Adsorption energies give evidence of substantial interactions between the two entities. The nature of the van der Waals bonding interactions that contribute to the efficient adsorption of Xylazine is further elucidated by the utilization of the Reduced Density Gradient (RDG) and Density Overlap Region Indicator (DORI), combined with Quantum Theory of Atoms in Molecules (QTAIM) investigations.

These findings provide insight on the potential of carbon-based nanomaterials in environmental applications, particularly with regard to the problem of drug contamination in water systems. The findings of this study have ramifications that extend to the enhancement of the design of adsorbents for the purpose of reducing pollution caused by pharmaceuticals.

References

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