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THE USE OF CARBON NANOTUBES FOR PESTICIDE MITIGATION

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RESUMO

Agricultural pesticides, chemical substances designed to eradicate pests in crops, are essential for enhancing food production. However, their use has significant negative impacts on fauna, flora, and human health, resulting in diseases, deaths, and undesirable environmental effects. Faced with this reality, driven by the growing demand for food on a large scale and population increase, the use of these pesticides is on the rise, leading to their accumulation in the environment and the food chain. The presence of these substances is detected in animal products and even in breast milk. Thus, research aimed at minimizing the impacts of agricultural pesticides and/or reducing their effects after use represents a crucial scientific strategy to sustain agricultural production and mitigate their harmful effects on the environment.In this context, the present study aims to investigate whether single-walled carbon nanotubes functionalized with COOHs can be used as adsorbents/filters for pesticides, specifically glyphosate, one of the most widely used and least toxic on the planet. Computational calculations were conducted within the semi-empirical method using the Maestro-Schrödinger, MOPAC2016, and Jmol programs to analyze the structural and electronic variations of the functionalized CNTs in the presence of glyphosate.The results revealed that increasing the concentration of OH and COOH groups in the CNTs resulted in a monotonic decrease in the heat of formation for the CNT-OHx and CNT-COOHx systems, both individually and in the presence of glyphosate (CNT-OHx+Gli and CNT-COOHx+Gli). Remarkably, the functionalized CNTs in the presence of glyphosate showed lower heat of formation, with the CNT-COOH25+Gli system proving to be the most stable among those studied, due to its lower total energy, reflecting greater entropy of the system. Additionally, COOH functionalization was found to be more effective in glyphosate adsorption than OH functionalization, demonstrating a significant improvement in the adsorption capacity of the nanotubes after chemical modification. These findings highlight the promise of functionalized carbon nanotubes as glyphosate adsorbents, with important implications for environmental remediation and public health protectiont.

PALAVRAS-CHAVE: single-walled carbon nanotubes, glyphosate, quantum mechanics, semiempirical method

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