

Which is superior for the absorption of the Lindane pesticide, graphene or graphene oxide? Experimental and DFT investigation

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Graphene and graphene oxide are intriguing materials with numerous applications, including adsorption, formulation of the composite materials, sensors, photovoltaics . . . [1-3]. In this study, graphene oxide is synthesized by reducing graphene oxide (with ascorbic acid) employing the well-established Hummers method, which may be summed up as the controlled treatment of graphite flakes with potassium permanganate in concentrated sulfuric acid. Combining FTIR and UV-VIS spectroscopy, the produced materials are characterized.

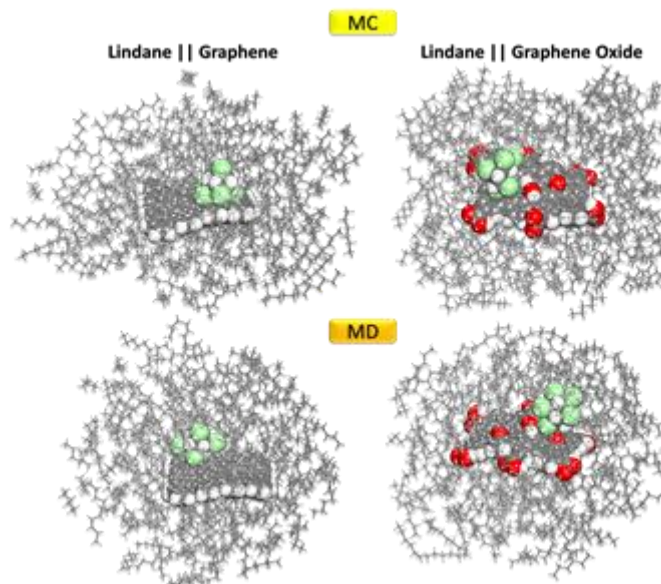


Figure 1: The final Molecular Dynamic (MD) and Monte Carlo (MC) geometries for Lindane adsorption onto Graphene and Graphene Oxide.

Lindane is adsorbed from hexane using a solution of concentration ranges from 25 to 500 ppb with a constant mass of 15 mg graphene or graphene oxide as adsorbents. The GC-ECD was used to determine the adsorbed concentration of Lindane. These materials have exceptional absorption characteristics. Graphene can remove up to 92.5 % of Lindane from hexane solution, whereas graphene oxide can remove up to 56.1 %. To gain a better understanding of the nature and adsorption energetics for the Lindane's interaction with the two adsorbents, quantum and molecular mechanics-based computations were undertaken (Figure 1).

References

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