Abstract
Nanomaterials have been demonstrated to be very effective adsorbent for various impurities because of their large volume-to-surface area and high adsorption potential. This research elucidates the attempt of designing computational model and procedure to access the maximum possible load of endosulfan, a persistent insecticide, on graphene nanosurface. We, here, present a strategy to calculate the maximum area covered by a molecule of endosulfan based on shape and its orientation on graphene surface. We have also modified the popular Langmuir’s model to calculate the maximum adsorbate load on adsorbent by including steric hindrance caused by a adsorbate molecule to others due to shape and adsorption configurations.

References

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Index Terms

Computer Science Artificial Intelligence

Keywords

Graphene Endosulfan Langmuir’s Model Steric Hindrance