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

- Kopecky F, Kaclik P, Fazekas T. Laboratory manual for physical chemistry. Farmaceutical faculty of Comenius University, Bratislava, 1996.

Index Terms

Computer Science
Artificial Intelligence

Keywords
Graphene  Endosulfan  Langmuir’s Model  Steric Hindrance