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THE STUDY OF DENSITY FUNCTIONAL THEORY ON SELECTED FUNCTIONALIZED MWCNTs AS ADSORBENT OF METHYLENE BLUE

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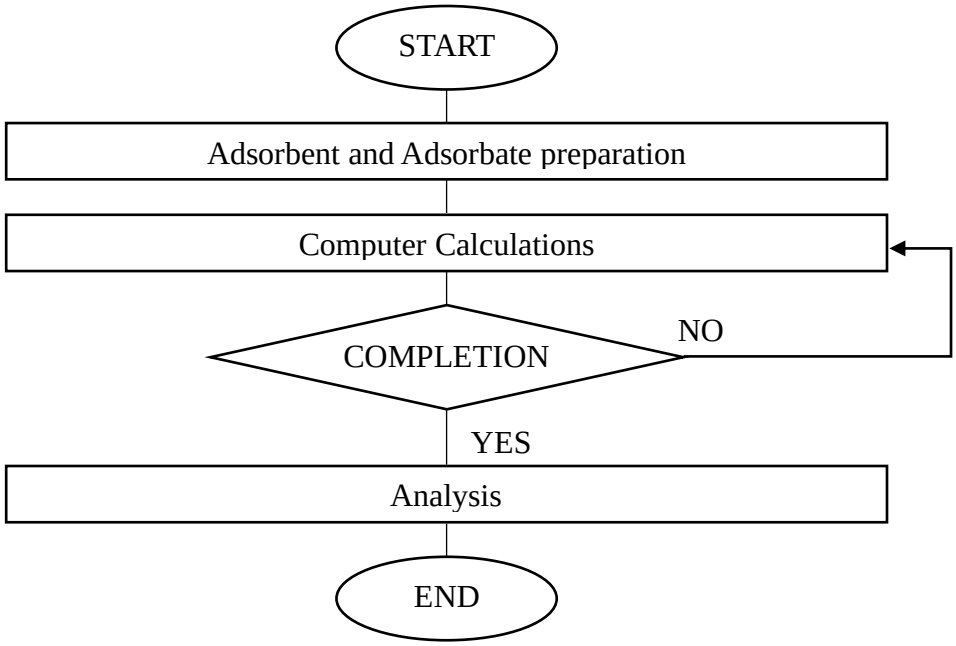
Abstract:
MB is a common dye that is found in wastewater dyeing and highly toxic to the environment. In order to remove MB, the adsorption by the MWCNTs membrane and functionalized MWCNTs are required as it is an effective way to remove dyes. To study the electronic properties, mechanism and selectivity interaction between MWCNTs and MB, a DFT method will be performed. The simulation was done in the Gaussian 03W software package. By using the DFT method, B3LYP with 6-31G(d) was used as a basis set for geometry optimizations. The selected functionalized MWCNTs used in this study were MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl. The B3LYP method with 6-31+G(d) basis set was used for energy calculations. The result showed that the electronic properties of MB with MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl were electrostatic attraction and hydrogen bonding. The mechanism of the MB with MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl were depend on the functional group that was introduces to the surface of MWCNTs. The energy value was found that acyl chloride functional group has the lowest energy value followed by carboxylic acid and hydroxyl. However, the most polarity functional group was carboxylic acid. The selective interaction between MB with MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl were at the distance where larger energy value occurred. The distance for MB with MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl were 1.36 Å, 2.0 Å and 2.377 Å respectively. The more negative the energy value, the stronger the interaction between MB and selected functionalized MWCTs.

***Keywords*:**
DFT, MWCNTs, Methylene Blue, Adsorption

Objectives:

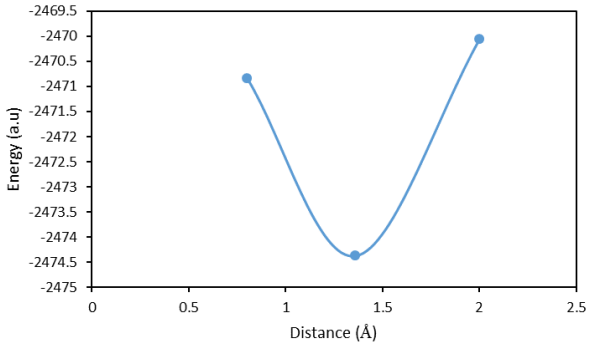
- To determine the electronic properties of selected functionalized MWCNTs using DFT method
- To identify the mechanism and selectivity of interaction between selected functionalized MWCNTs with MB

Methodology:

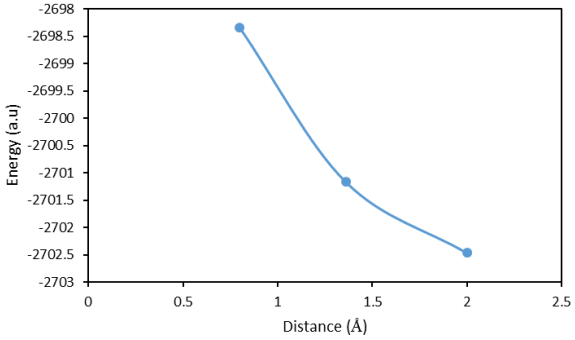


Results:

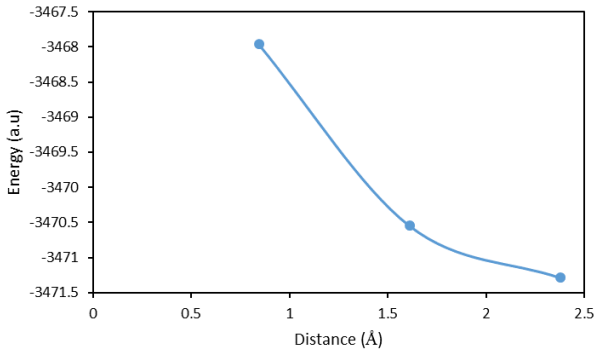
Interaction between MWCNTs-OH and MB



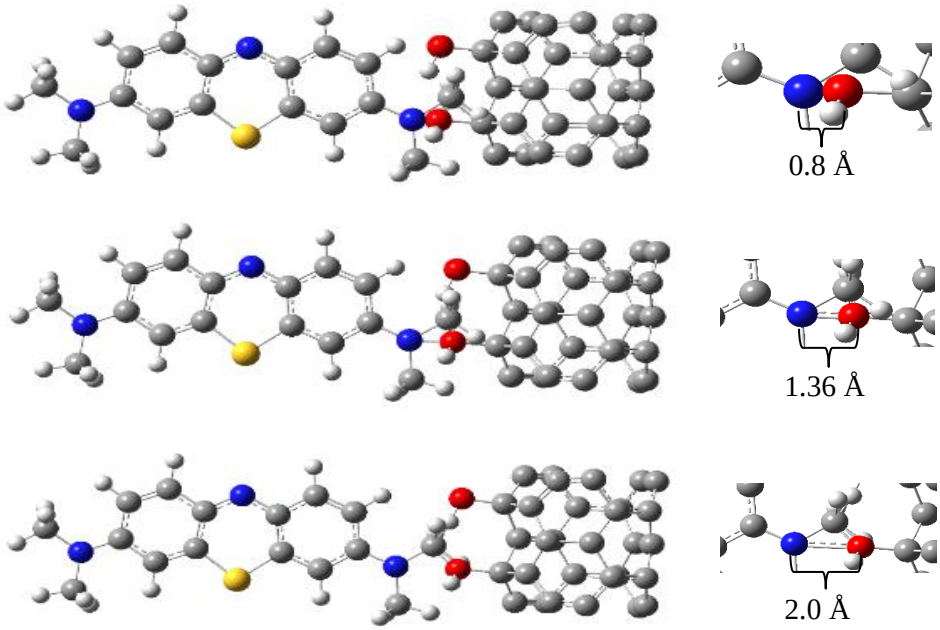
Interaction between MWCNTs-COOH and MB



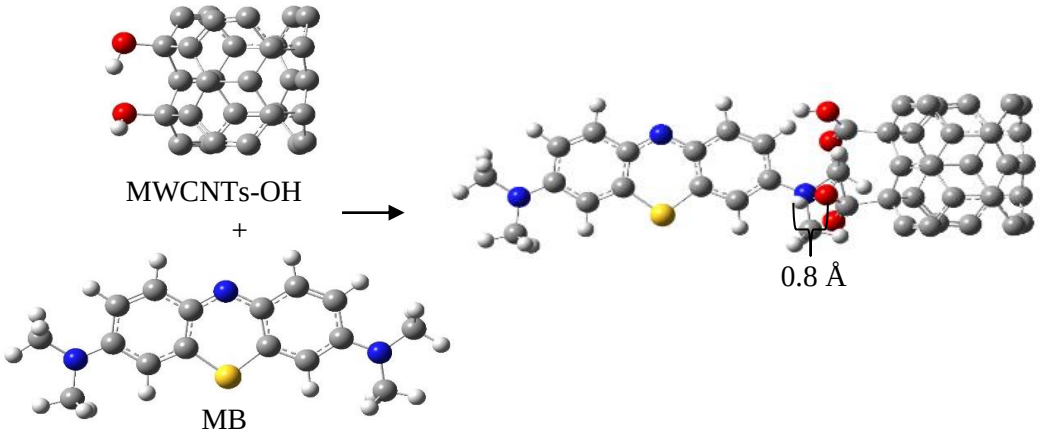
Interaction between MWCNTs-COCl and MB



Electronic properties of optimized MB and MWCNTs-OH



Mechanism of MB with MWCNTs-OH



Conclusion:

The study of density functional theory on MWCNTs-OH, MWCNTs-COOH and MWCNTs-COCl as adsorbent of methylene blue was performed. It was found that the interaction between MWCNTs-OH with MB is an electrostatic attraction with energy of -2474.3715 a.u and RMS value of 6.545. While for MWCNTs-COOH with MB, the interactions are an electrostatic attraction and hydrogen bonding with energy of -2702.4664 a.u and RMS value of 5.461. The interaction between MWCNTs-COCl with MB is hydrogen bonding with energy of -3471.2873 a.u and RMS value of 5.011. The mechanism of MB with functionalized MWCNTs was depends on the functional group that is introduce on the surface of MWCNTs. The functional group that has high polarity was carboxylic acid functional group. The selective interaction between MB and functionalized MWCNTs was at the distance where the energy value was at the lowest. The more negative the energy value, the strong chelating interaction between MB and functionalized MWCNTs.