Investigation of Interaction between Carbon Nanosheets with air Pollutants by DFT method

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Today, environment pollution has become an important issue. Environmental pollution is mainly caused by pesticide pollution of air, water and soil caused. The results of this contamination is not only destroying biodiversity, but also endanger human health. Nano technology has many advantages in environmental technology improvement and provides new useful technology. Graphene is a two-dimensional crystalline material which has been identified and analyzed recently. The new material has many unique features. In this project, the interaction between carbon nanosheet (10.0) and 2-hydroxy-1-phenyl athanone has been performed by DFT (B3LYP) method and 6-31 G (D) basis set at at 298 K and 1 atm and electronic and mechanical properties of formed complexes has been studied.As the results show, the chemical adsorption is not performed thermodynamically and the best interaction is physical adsorption.

Keywords : keywords: Nanotechnology, Nano sheet, Graphene, 2-hydroxy-1-phenyl ethanon

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