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Hazards of PAH and use nanomaterial for eliminate contaminants

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EDITORIAL NOTE

PAHs (polycyclic aromatic hydrocarbons) are a category of over 100 compounds produced by incomplete combustion of coal, oil and gas, waste, or other organic compounds such as tobacco or charbroiled meat. A few PAHs are utilised in the production of pharmaceuticals, colours, plastics, and insecticides. Polycyclic aromatic hydrocarbons have been blamed for the rise in lung cancer rates. Some ways for removing contaminants from the environment include decomposition by bacteria (Geobacillus), use of Eisenia Fetida earthworms, phytoremediation, and use of Zeolite, among others. Single-walled carbon nanotubes (SWNTs) have been employed to minimise and eliminate organic contaminants from the environment for the past ten years [13,14]. Organic compounds bind to SWNTs, making them effective sorbents. Some ways for removing contaminants from the environment include decomposition by bacteria (Geobacillus), use of Eisenia Fetida earthworms, phytoremediation, and use of Zeolite, among others. Single-walled carbon nanotubes (SWNTs) have been employed to minimise and eliminate organic contaminants from the environment for the past ten years [13,14]. Organic compounds bind to SWNTs, making them effective sorbents. SWNTs were simulated and analysed in this study to recognise, remove, and modify polycyclic compounds. A romatic hydrocarbons (Anthracene) into less hazardous hydrocarbons. Arrangements Carbon nanotube sensors also have a high sensitivity. Possible capabilities for environmental monitoring an poisonous and hazardous compounds can be easily developed. Polycyclic aromatic hydrocarbons (such as anthracene, benzo[a]pyrene, and others) are non-polar, non-ionized hydrophobic chemicals. In water, they are just weakly soluble. They are extremely hazardous to the environment. Anthracene is removed and converted to low-risk compounds using single-walled carbon nanotubes (SWNTs). At the level of B3LYP/6-31G, electron transport between anthracene and SWNT is investigated using a density functional method. SWNT is particularly sensitive to the presence of anthracene molecule, according to the electronic properties calculations. The variations in HOMO/LUMO and gap energy (Eg) were significant. The DFT approach was used to calculate the thermodynamic parameters.