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Theoretical study of the adsorption energy of some linear saturated hydrocarbons on SWCNT: DFT calculations HEWA ABDULLAH, HASSAN H. ABDALLAH, Computational Nanoscience Lab, Research Center, Salahaddin University, 44001 Erbil, Iraq — Carbon nanotubes represent one of the building blocks of innovation across most industries. Carbon nanotubes have many applications based on the aspect ratio, mechanical strength, electrical and thermal conductivity of these nano materials. In this study the adsorption of a single molecule of the some linear saturated hydrocarbons inside and on the surface of a tube of single-walled carbon nanotubes (SWCNT) was investigated using Density Function Theory (DFT). The results showed that all guest molecules prefer to be adsorbed into the surface of SWCNT rather than into the CNT tube. Upon adsorption of the guest molecules, the energy gap was considerably reduced, resulting in improved electrical conductivity. DOS and NBO analysis were performed to discover intermolecular interactions. Chemical reactivity was investigated in terms of chemical hardness, softness and absolute electronegativity

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