RESEARCH STUDY OF NOTICING UNSAFE PESTICIDES - PARTICLE ADSORPTION ON PRISTINE SINGLE-WALLED CARBON NANOTUBES

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ABSTRACT:

A computational study, density functional theory (DFT) have been applied on the adsorption of DDD, DDE and DDT molecules on (8,0) pristine single-walled carbon nanotubes (PSWCNTs). The DDD, DDE and DDT molecules adsorption are aggressively favorable with adsorption energy (Eads) equal to -67.266, -58.776 and -52.245 eV respectively. In this study, the electronic properties analysis reveals that the physisorbed DDD, DDE and DDT are changing the highest occupied molecular orbital (HOMO) energy gap and lowest unoccupied molecular orbital (LUMO) energy gap of carbon nanotubes which have been reduced after interaction with these molecules from 0.519 eV to 0.356, 0.289 and 0.296 eV respectively. These three insecticide molecules make changes outside of the carbon nanotube to the set of energy molecule and thus nanotubes are obtained as conductive structure. As inference it reveals that the pristine single-walled carbon nanotubes can be a good sensor for the detection of DDD, DDE and DDT molecules.

Keywords: HPLC, PDA, stability indication method, drug.

1. INTRODUCTION:

Since the discovery of carbon nanotubes CNTs in 1991, it has been intrigued broad interdisciplinary"courtesies."CNTs and nanoparticles with low dimension and high aspect ratio "surface-to-volume ratio are presenting unique physical, chemical, mechanical and permanent electrical properties"[1–3]. CNTs and nanoparticles have a wide range of important applications including nanoelectric devices, energy storage, and catalyst [4-6]. They can detect even a small concentration of the analyze, they can be utilized in chemical and biological sensors"[1-7]."CNTs can be either single-walled (SW) with discrete fragment of curved carbon sheet, or multi-walled"(MW)."They can be either metallic or semiconducting dependent

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on their chirality defined with a pair of integer indices (n, m)"[8]."CNTs can be classified to armchair (n, n), zig-zag, (n, 0) and chiral (n, m)."The armchair nanotubes always show a metallic behavior with high current capacity and the ballistic nature of electron transport. They always maintain metallic property and mechanic stability under the compressive and tensile strains. Thus, the current variation in the armchair nanotube is more stable under small uniaxial strains, and this characteristic could be applied to thermal strain"[9]. So armchair SWCNT based chemical sensors are effective devices to detect various molecules. Fast response time and high sensitivity at room temperature are the most important characteristics of these sensors to detect contaminant molecules"[10]. "SWCNTs cannot detect some gaseous molecule such as carbon monoxide or ammonia because of the weak Van der Waals interaction and insufficient charge transfer between SWCNT surface and molecules. Limited environmental sensitivity of pristine CNTs which results from smooth surface low adsorption energy, affinity and long recovery time could be modified by functionalization. Chemical modification is an effective approach to overcome this restriction and improve the binding strength by the enhancement of the chemical reactivity of SWCNTs. Although the electronic properties of CNTs are strongly depends on the delocalized p-electron conjugation system that make the CNTs electrochemically active [11]. Use of insecticides in agriculture is a common practice over the whole world. These insecticides or pesticides help to increase agricultural productivity by killing insects selectively. However, they can have some serious hazardous effect on human body as well. One such widely used insecticide is dichlorodiphenyltrichloroethane"(DDT)."Because of its adverse effect on environment [12-14], use of this pesticide has been banned in many countries. But DDT has been still found to be contaminating agricultural soil and water in many places. It further exhibits very slow degradation rate, which can take upto 30 years. By getting accumulated in plants and animals, DDT can further show bio magnification effect as we go up in a food chain [15]. Its metabolites dichlorodiphenyldichloroethane"(DDD) and dichlorodiphenyldichloro ethylene (DDE) and both are equally harmful to human body.

2. RELATED STUDY:

Titanium dioxide (TiO2) is one of the most widely investigated photocatalytic materials that can be used in the decomposition of volatile organic compounds, advanced oxidation processes for wastewater and bactericidal treatments, window glass self-cleaning for green intelligent buildings, dye-sensitized solar cells, solid-state semiconductor metaloxide solar cells and self-cleaning glass for photovoltaic devices [1-3]. TiO2 decomposes the organic pollutants settling on its surface when irradiated with UV light turning the surface to be hydrophilic [4]. Hydrophilic TiO2 thin films have the characteristics of spreading water out on its surface, thus carrying dust particles away while flowing down the surface. Therefore, the photocatalytic characteristics combined with the hydrophilic properties of TiO2 makes it an excellent self-cleaning surface that attracts worldwide attention for many applications to save time and cost with regular cleaning methods [5]. Several coating processes have been proposed to prepare uniform TiO2 coatings. Liu et al. [6] prepared titanium thin film by sol gel method. Abdulraheem et al. [7] successfully synthesized TiO2 thin films by electron beam assisted physical vapor deposition. Da Silva et al. [8] used microwave heating to prepare thin TiO2 films. Nevertheless, low-cost controllable solution-based processes for preparation of TiO2 thin films are highly desirable. Recently, Xi et al. [5] proposed an efficient and easy to scale up coating method for uniform and homogeneous TiO2 thin films for self-cleaning applications. Their method relies on developing a solution-based adsorptive self-assembly approach to fabricate anatase TiO2 thin films on glass substrates. They were able to tune the number of process cycles to increase the film thickness into the desired value. Moreover, the as-prepared nanostructured TiO2 thin films on glass substrate did not cause deterioration of the optical transmission of glass; instead, they improved optical performance of commercial solar cells over a wide range of incident angles of light which is a very critical factor for self-cleaning of optical devices and solar panels. In this work, we report on the use of two TiO2 nanocolloids

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prepared via polyol method starting from two different titanium precursor salts and characterized by transmission electron microscopy (TEM). The coating films were deposited via adsorptive self-assembly method [5] and characterized by scanning electron microscopy (SEM), ellipsometery, atomic force microscopy (AFM), optical microscope, UV-vis, contact angle and surface tension measurements. Moreover, the effect of soiling on the transmission properties of the coated glass was studied for self-cleaning application of solar panels under desert conditions.

3. PROPOSED METHODOLOGY:

Two TiO_2 nanocolloids were prepared by polyol method as described in details in [9-11]. Starting with about 2.7 g of each of two precursor salts: Titanium (IV) oxysulfate ($TiOSO_4$, Sigma-Aldrich 99%) for coating 1 (TC1) and titanium isopropoxide ($Ti(OCH(CH_3)_3)_4$, (Sigma Aldrich, 95%) for coating 2 (TC-2) that were measured and introduced into a three-neck flask and stirred for 30 min to dissolve in tetraethyleneglycol (TEG) from (Sigma-Aldrich, ≥ 99%) at room temperature. To control the particle size of the synthesized nanoparticles, 2.9 g of sodium hydroxide pellets were dissolved in 5 mL of deionized water and the solution was gradually added to the mixture using a syringe. The mixture was mechanically stirred and heated at a rate of 6 °C min^{-1} from room temperature to 165 °C under reflux for 3 hours. At this stage, TiO_2 nano-colloids were synthesized.

To validate the effects of DDD, DDE and DDT molecules adsorption on the nanotube, electronic properties, electronic density of states (DOS) of the nanotube and adsorbate/nanotube complexes were calculated"(Fig. 3)."For all three configurations, it can be found that DOS are not affected by the DDD, DDE and DDT adsorption"(Fig. 3). So, the Eg of the nanotube has no significant change externally (DDD adsorptions Eg = 0.356 eV, DDE adsorptions Eg = 0.289 eV and DDT adsorptions Eg = 0.296 eV). This occurrence is expected to bring about obvious change in the corresponding electrical conductivity because it is well known that the energy gap or band gap in bulk materials is a major factor determining the electrical conductivity of a material and a classic relation.

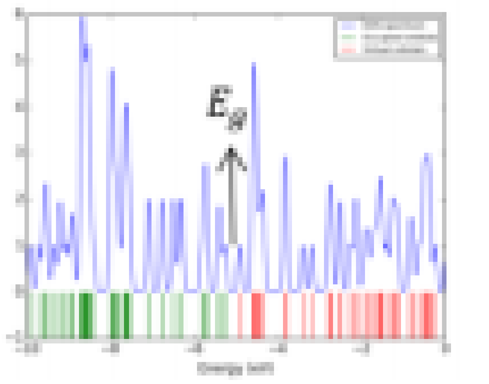

Fig.3.1. Proposed system results.

5. CONCLUSION:

This work has been performed a computational study of density functional theory (DFT) calculations to study the electronic properties of DDD, DDE and DDT molecules which are adsorbed in the surface of pristine carbon nanotube. It was found that the three molecules can be strongly adsorbed in the nanotube exterior surface with high adsorption energies, and changes energy gap which leads to increase the electrical conductivity. Charge transfer between the molecule and CNTs generates the sensing property of the CNTs. Importantly, it was deduced that the pristine carbon nanotube can acts as a good sensor for DDD, DDE and DDT molecules.

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