Abstract

The major objective of this study is systematically to investigate various electronic properties of the 1-D nanomaterials (SWZCNTs, SWZBNNTs, SWZZnONTs, and SWCMoS$_2$NTs), which are used as a carrier to altered anticancer drugs (5-FU, CH, CY, HY, and OX). All of our investigations are based on first principle Density Functional Theory (DFT) calculations. After calculating the electronic properties of these anticancer drugs, all these anticancer drugs have insulation behaviors, but CY has a semiconductor behavior. Furthermore, these anticancer drugs had a greater interaction with other structures because of their lower and higher value of the chemical potential.

First of all, the ((6,0), (7,0), and (11,0)) SWZCNTS and SWZBNNTs utilized as a career to (CH, CY, and 5-FU) anticancer drugs. The complexes structures have electronic band gap less than the pristine of these tubes. By adsorbing the same anticancer drug on the SWZCNTS and SWZBNNTs, It was found that the anticancer drug/SWZBNNTs have interesting results compared with SWZCNTS. Moreover, the anticancer drug/SWZBNNTs is more stable compared with anticancer drug/SWZCNTS. The adsorption energy is increasing by increasing the diameter of the tube, which is utilized to deliver these anticancer drugs, except the 5- FU/(7,0)SWZBNNTs has an opposite behavior. Then, it was recognized that the (11,0) SWZBNNTs are the best substrate to deliver the CH anticancer drug, due to it has a higher value of the adsorption energy E_{ads} compared to others. In brief, we detected that the SWZBNNTs is the best substrate to deliver these anticancer drugs compared with SWZCNTs.

Various diameters of the $(n,0)$ SWZZnONTs and (n,m) SWAZnONTs (where n=m ; from 8 to 12) are used to deliver HY anticancer, which is located in inner and outer of these tubes. For inner locations, the HY/(12,0) SWZZnONTs has a higher stability compared with others HY/SWZZnONTs tubes and still has asemiconductor behavior. That means this anticancer drug became more stable when sited it on the higher diameter of the tube. So, this result confirmed by using the SWAZnONTs. Moreover, it was detected that all complex structures in the inner sites are required a smaller excitation energy to transfer electrons because of the chemical hardness of the HY/(SWZZnONTs or SWAZnONTs) is increased. For outer sites, it was found that the opposite behavior, excepted the HY/(12,0) SWZZnONTs and HY/(10,10) SWAZnONTs have the reverse behavior. The HY anticancer drug has a weak interaction with ZSWZnONTs and SWAZnONTs because of there is the lower value of the electrophilic index, but the HY/(10,0) SWZZnONTs and HY/(11,11) SWAZnONTs have a higher value of the

electrophilic index, which led to make a good interaction between them. Then, the (12,0) and (12,12) are the best substrate to carrier the HY. Another interesting work is examined by utilizing (3,2) and (4,2) SWCMoS$_2$NTs to deliver OX anticancer drug with and without various impurities and sites in different distance between them. The complex structure (OX/(3,2)SWCMoS$_2$NTs) has a semimetal behavior with a direct transition of electrons at Γ point. There are very interesting results by changing the S atom by P or Ga impurities. So, the (OX/p-doped (3,2) SWCMoS$_2$NTs) structure has a n-type semiconductor behavior when the distance between OX anticancer drug and p-doped (3,2)SWCMoS$_2$NTs is 1.76 Å compared with other distances. By utilizing Ga impurity, the best results are detected at 1.42 Å and the behavior is became p-type behavior and more stable compared to others. For (OX/(4,2)SWCMoS$_2$NTs) has metal behavior. By using P impurity at different distance, the behavior is changed from metal to semi-metal with direct transition at Z point. The behavior of this complex structure is became n-type semiconductor at 1.76 Å.. The stability of all complex structures with Ga impurity is more stable compared with P impurity. In brief, the best substrate of the (3,2) and (4,2) SWCMoS$_2$NTs can be utilized to career OX anticancer drug when we used Ga impurity compared with P impurity.