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Homo-Lumo, Density of States Studies of SnO2 Doped with Single Layered Graphene

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ABSTRACT

The quantum chemical investigation of single-layer graphene combined with SnO_2, focusing on its structural characteristics. The structural and geometrical parameters of the graphene were analysed using the B3LYP/6-31+G(d,p) basis set. Electronic transitions were calculated in a water environment using DFT/ B3LYP/6-31+G(d, p), which revealed charge transfer within the molecule. Additionally, we examined the molecular electrostatic potential (MESP). The HOMO-LUMO analysis provided detailed insights into the charge transfer density between acceptor and donor groups in the graphene-SnO_2 system. The density of states (DOS) of the single-layer graphene was also studied.

Keywords:— *MESP. HOMO-LUMO, DOS*

I. INTRODUCTION

Various methods have been developed for graphene preparation, including micromechanical exfoliation, epitaxial growth, chemical and electrochemical reduction of graphite oxide, and bottom-up organic synthesis [1]. The remarkable physical properties of graphene, including quantum electronic transport, extremely electromechanical modulation, and high surface area, make it an ideal substrate for forming hybrid structures with a variety of nanomaterials. One promising approach to harness these properties for applications is to incorporate graphene sheet hybrids with metals, metal oxides, and polymers [2,3]. Tin oxide (SnO_2) is recognized for its outstanding optical, gas sensing, and photocatalytic properties [4]. Many semiconducting metal oxide nanoparticles are considered efficient photo catalysts for eliminating hazardous organic pollutants [5].

Synthesis of Go-SnO_2 Nanocomposite

Grapheneoxide(GO) was synthesized by the Modified Hummer's method [6]. 100 mg of GO was suspended in100 ml of H_2O and ultrasonicated for 2h. In a typical experiment, 1m mol $SnCl_4 \cdot 6H_2O$ and 2m mol urea were separately dissolved in 25 ml water. Then these urea and $SnCl_4$ solutions were slowly and sequentially added to 50 ml of graphiteoxide suspension under stirring.

II. MOLECULAR STRUCTURE AND STRUCTURAL ANALYSIS

The optimized molecular structure single layer graphene and SnO_2 were calculated by B3LYP at basis set 6-31G(d, p) method[5] are shown in figure 1. X-ray diffraction (XRD) patterns of SnO_2 nanoparticles and graphene-SnO_2 nanocomposite are shown in

figure 1. The diffraction peaks of SnO_2 and graphene-SnO_2 composite clearly show the tetragonalrutile structure (JCPDS No. 41-1445) confirming that the synthesized and the rmallytreated samples retain the tetragonal SnO_2 structure.

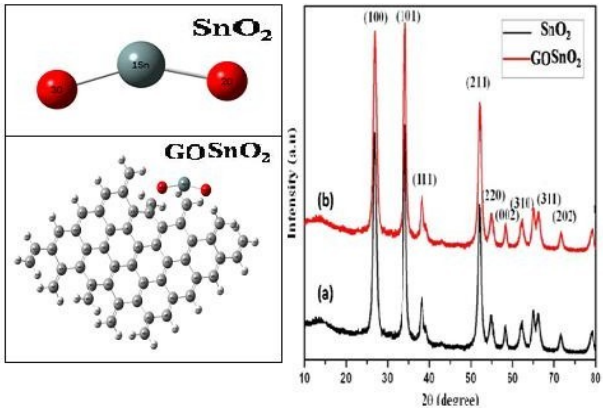

Figure 1: Molecular Structure and XRD Peaks SnO_2 and $GOSnO_2$

The strong intensity can be attributed to the good crystallinity of SnO_2 particles. The diffraction peaks of SnO_2 nanoparticles, and graphene-SnO_2 nanocomposite are indexed with (100), (101), (111), (211), (220), (002), (310), (311) and (202)planes.The absence of specific diffraction peaks of graphene may be due to the disordered interfacial structure produced by the interfacial bonds between SnO_2 nanocrystals and graphene sheets[6-8].

Molecular electrostatic potential and density of states

The molecular electrostatic potential (MESP) of the SnO_2 and GO-SnO_2 of the molecule is shown in figure 2. The MESP of the compound predicting molecular reactive behaviours of various biological systems and its hydrogen bonding inter action of titled of the molecule.

Electrostatic potential maps illustrate the charge distributions of molecules three dimensionally. The red colour denotes the region of electronegative and green denotes electropositive region. The molecule is more electronegative to wards the SnO_2 substituted area than carbon atoms.

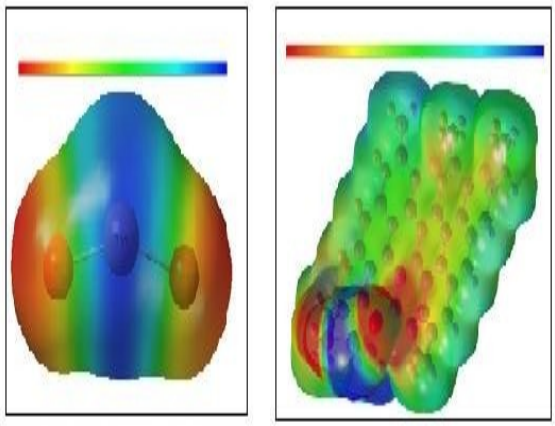

Figure 2: Density of States of SnO_2 and GO-SnO_2

Homo-Lumo Analysis.

The HOMO-LUMO has been used to prove the bioactivities from intra molecular charge transfer with in the molecules [9.10]. The energy values of HOMO orbital and LUMO orbital were lying at an energy value of -0.1380 au and 0.09517 au respectively. The electron charge transition takes place from HOMO orbital to LUMO orbital and this energy transition implies charge transfer from C=C to C-C of the title of the molecule. The HOMO-LUMO energy gap was obtained at 0.23317 au in the isolated gas molecular calculations.

The Frontier Molecular Orbital gives an idea about the reactivity of the molecule and the active site can be demonstrated by the distribution of frontier orbital. The HOMO-LUMO frontier orbital compositions for calculated with the DFT/6 -311G orbital energy level are shown in Figure 3 respectively. In order to evaluate the orbital energy level behaviour of the title compounds, the third highest and highest occupied MO′s (HOMO and HOMO -3), the lowest and the third values lowest unoccupied MO′s (LUMO andLUMO+3) are performed and energy band gap values were observed.

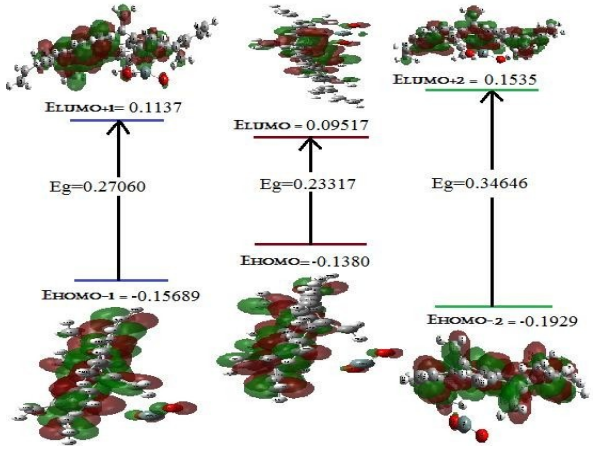

Figure 3: Density of States of SnO_2 and GO-SnO_2

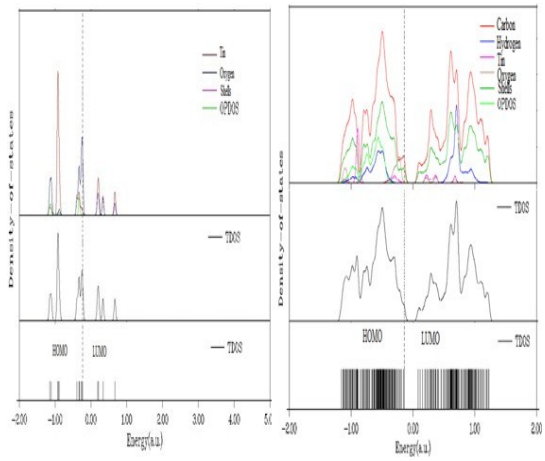

Figure 4: Density of states of SnO_2 and GO-SnO_2

Density of States

The DOS plot results show that population in the molecular orbital from figure 4. The OPDOS result shows that nonbonding, bonding and anti-bondinginter actions between the two orbital atom groups. The positive value of OPDOS indicating that the bonding interaction and negative value indicates the anti-bonding interactions and zero values indicates the nonbonding interactions. The DOS plot gives the composition of group of orbital contributing to the molecular orbital. The plot for DOS is taken from the range of-2.00 a.u.to+2.00a.u.

The graphexhibits the orbital characteristics of different energy range. It is the major contribution from s orbital and p orbital basic function of carbon in the frontier molecular orbital. The partial density of states (PDOS) of the carbon atom of the title of the molecule exhibits the total density state soft he molecules. The PDO Soft he carb on has just larger positive energy then the negative energy values. The OPDOS curve is in the negative region shows anti-bonding characteristic of the molecule.

IV. CONCLUSION

Grapheneoxide and graphene-tinoxide composite have been prepared by modified hummers method and chemical reduction methods respectively. GO-SnO_2 composite shows the is land like structure with the SnO_2 nano-particles coated on graphene sheets. The molecular electrostatic mapping and density of states were performed. The frontier molecular orbital energy diagram illustrates the occupancy of positive and negative energies.

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