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SYNTHESIZED AND CHARACTERIZATION STUDIES OF SINGLE LAYERED GRAPHENE

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ABSTRACT

Graphene has been prepared bymodified hummers method and chemical reduction respectively. The XRD result reveals graphite was oxidized to graphene oxide and graphene oxide was successfully reduced to hexagonal graphene. From FESEM and EDX results show the morphology of graphene shows wrinkled paper like structure. Graphene oxide paper, layered structure of paper with layer-by-layer stacked graphene oxide sheets is clearly observed. FTIR spectra result were confirmed the functional groups of Graphene layer. The UV-visible spectra were carried out in the wavelength regime of 400-800 cm^{-1}.The Raman spectrum of graphene, peak shift was observed towards the lower region compared to Graphene.

1 INTRODUCTION

After the invention of graphene by [1], it produced a great interest for graphene and its applications. Graphene is the favored medium by physicists and materials researchers, because of its simple arrangement and process capacity. For tentatively portraying the oxygen-containing bunches, computational techniques are of awesome offer assistance. Quantum computational techniques have turned into a promising device for the investigation of sub- atomic structure holding, compliances, steadiness and response instrument.

Quantum mechanical expectation of atomic properties [2] has its wide use in concoction issues, inferable from the advancement in PC equipment and productive computational programming. Gaussian is the most broadly utilized program bundle, for performing electronic structure figuring's. Numerous exploratory and hypothetical gatherings have indicated bunches of intrigue and

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clarified the way of holding and reactivity of the framework.

The majority of the clarifications depended on some natural thoughts and exact tenets that were basically gotten from a few exploratory perceptions and numerous compound responses. Hence, the need for a natural and right hypothetical approach for these ideas was inescapable. In this study, structural and confirmation properties of single layer graphene.

2 EXPERIMENTAL STUDIES

Graphite powder was obtained from Merck, sodium nitrate ($NaNO_3$), potassium permanganate ($KMnO_4$), hydrogen peroxide (H_2O_2), sodium hydroxide (NaOH), hydrochloric acid (HCl), double ionized (DI) water was used for all the reactions. GO was synthesized using the modified Hummers method. X-ray diffraction (XRD) were recorded at room temperature at the filtering rate of 0.02°/min for the range from 10° –80° utilizing PANalytical X'Pert-Pro diffractometer with Cu Kα1 radiation (λ=1.5406 A°). The infrared spectra of the examples were acquired by utilizing a Fourier change infrared (FTIR) spectrometer (Bruker Tensor 27, Germany) with a working range of 400 cm^{-1}-4000 cm^{-1} in a KBr pellet technique.

The Raman spectra were analysed using Peakseeker Raman spectrometer with excitation wavelength of 520 nm as a laser source with a extent up to 4000 cm^{-1}. The UV-visible spectra were carried out using JoscoV- 650 spectrophotometer in the wavelength regime of 400-800 cm^{-1}..A powder X-ray diffraction spectrum of single layered graphene was shown in figure 1. The diffraction peak of this molecule was found at 2θ=26.3° which corresponded graphite structure. The optimized molecular structure parameters such as bond length and bond angles of the single layer graphene were calculated by B3LYP at basis set 6-31G(d,p) method are shownin figure 1.

The SLG consists of carbon sp^2 hybridization of single and double bonding atoms. Generally, single C-C bonding in aromatic ring structure will not have the same bond lengths and bond angles. The presence of these peaks confirms the formation of graphene oxide[4]. The graphene oxide peak at 10.3° it is reduced to graphene. In addition, a new peak was observed at around 43.3° of (100) plane

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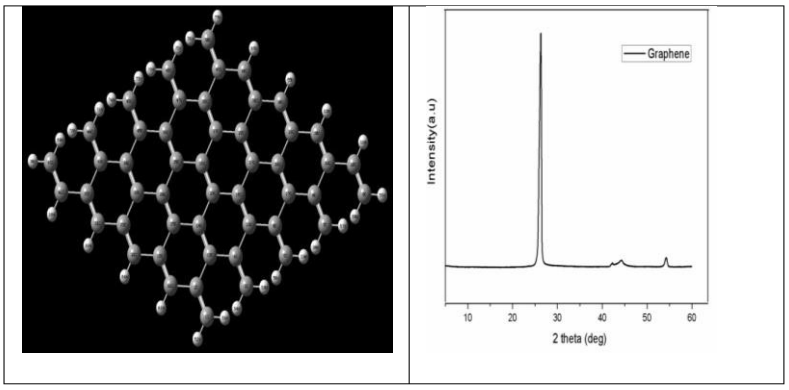
(JCPDS No. 75-1621). The other functional groups, impurities and amorphous carbon were removed by the chemical reduction process. The low crystallinity of graphene indicates the presence of residual oxygen-containing functional groups in the graphene sheets [4].

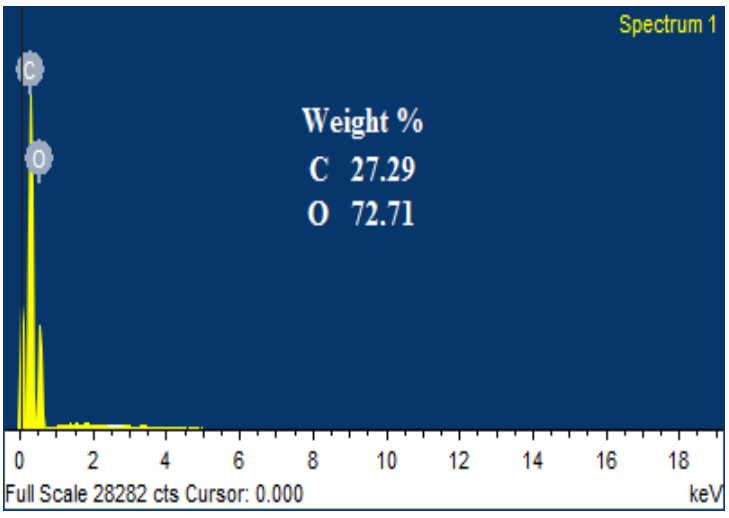
Figure 1 Molecular structure and XRD peak of SLG



3 FESEM and EDS Analysis

The modified Hummer‟s technique gives samples of good homogeneity and high purity. Composition analysis was done through EDS investigations of pure GO samples as shown in Figure 2.

Figure 2 EDS plot of Graphene



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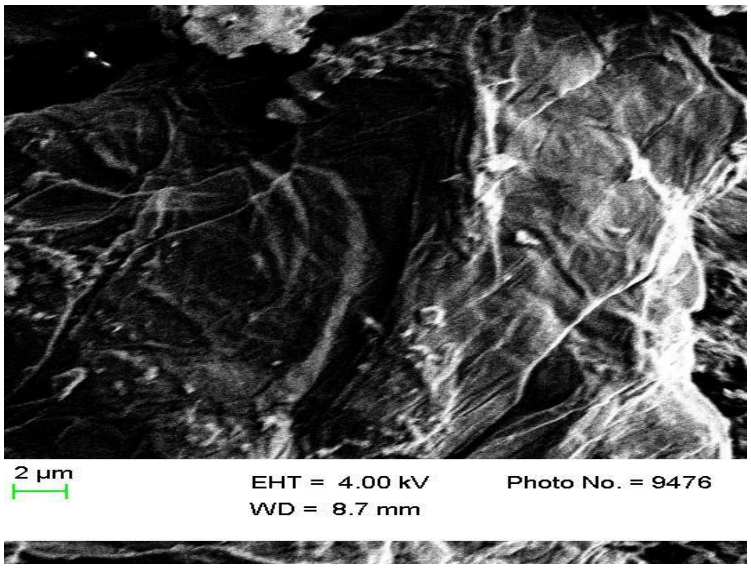
The morphology of graphene[5] shows wrinkled paper like structure. Graphene oxide paper, layered structure of paper with layer-by-layer stacked graphene oxide sheets is clearly observed. The weight percentage is presented in the inset tables for the as prepared samples. The atomic weight percentage is in good agreement with the composition.

Figure 3 FESEM plot of Graphene



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4. FTIR spectra of pure GO

The intensity of absorption peaks related to oxygen functional groups was decreased with the removal of other functional groups such as OH, COOH, C-O, C-O-C and impurities. The peak present in the wavelength range of strong aromatic ring C=C at 1563 cm^{-1} is related to the [4,6].

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Figure 4 FTIR spectra of pure GO

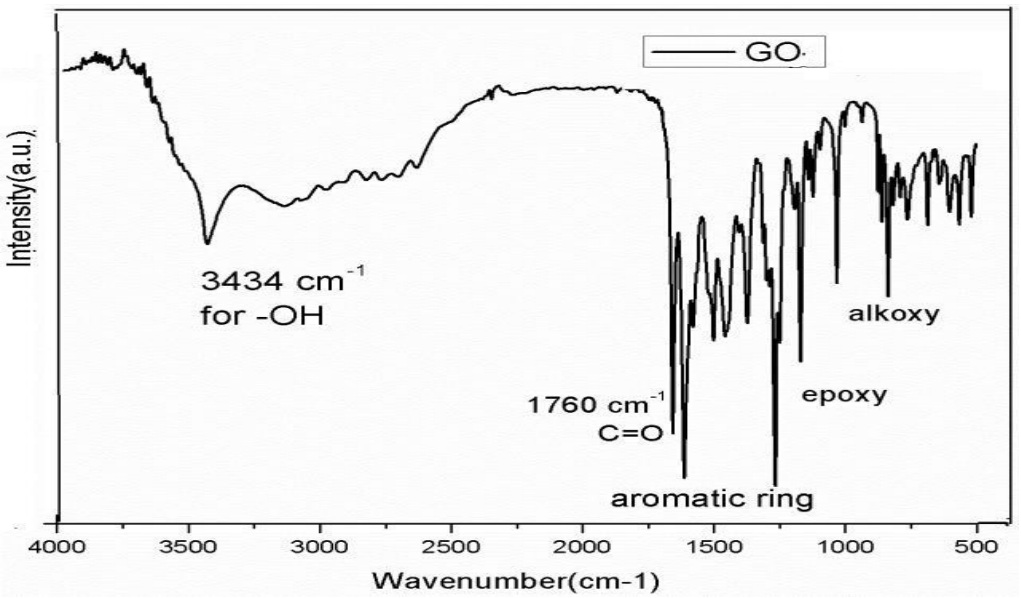
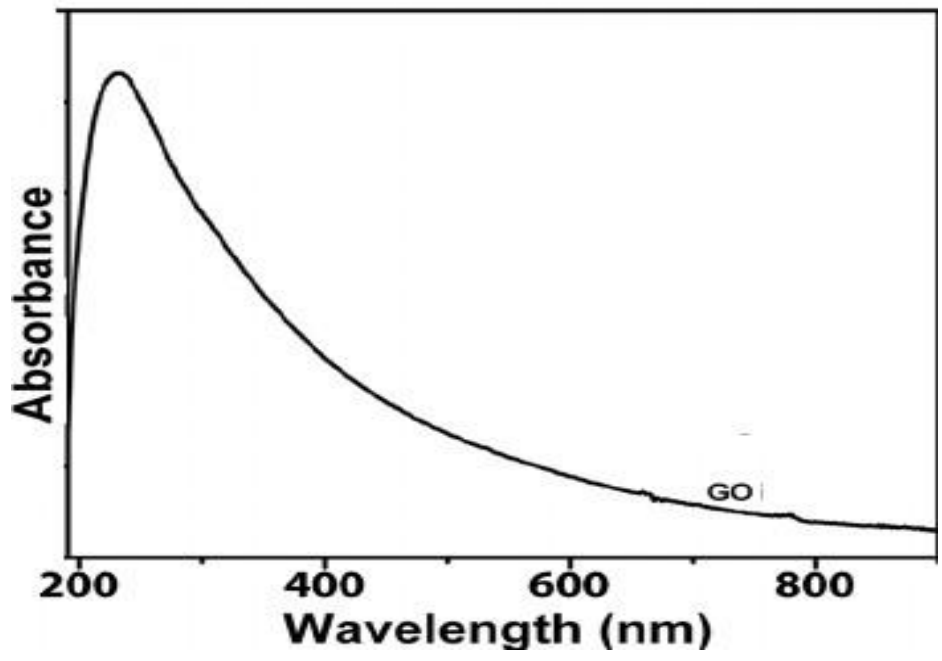


Figure 4 shows the FTIR spectrum of the GO composite, in which the absorption peak at 3433 cm_{-1} corresponds to the stretching vibration of OH. The aromatic ring of C=C formed at 1638 cm^{-1} is shifted to the higher wavenumber side.

5. UV -Vis spectra of pure GO

The UV-Vis absorption spectra of GO is shown in Figure 5. For GO, the broad absorptionpeak starts from 230 nm with the maximum absorption peak conversion of the aromatic C=C bond of GO [7]

Figure 5 UV -Vis spectra of pure GO



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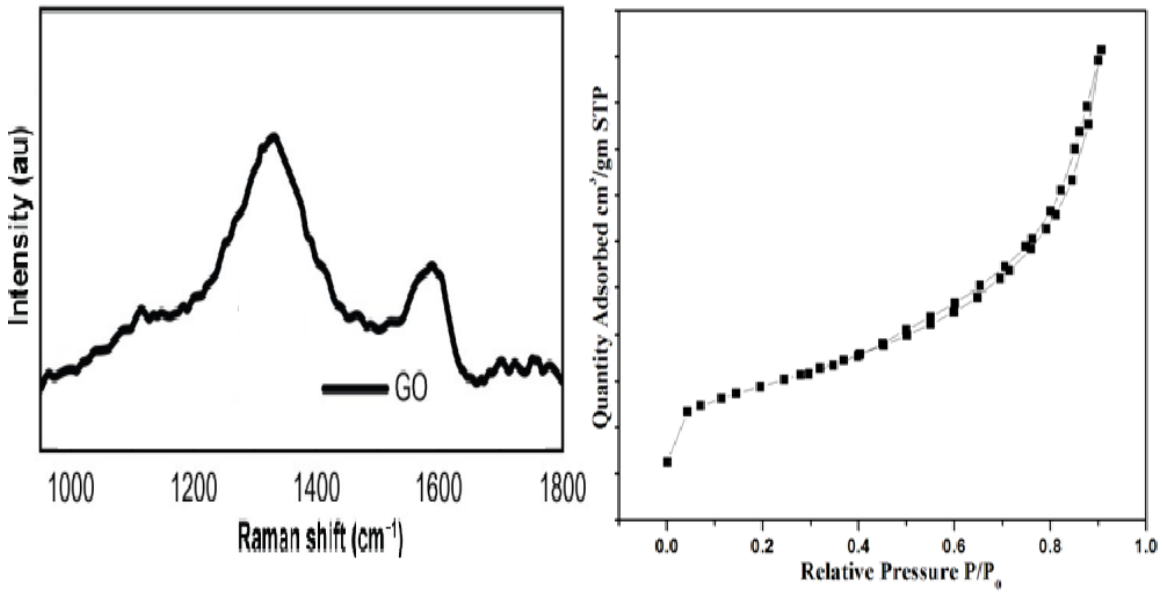
6. Raman, BET spectra of pure GO

Raman spectra of GO is shown in Figure 6. The Raman spectrum of GO shows the D band at1334 cm^{-1} due to the plane imperfection related to the breathing mode ofaromatic rings, k-point phonon of A1g and G band at 1586 cm^{-1}, which is recognized to be the plane vibration of an E2g phonon of sp^2 hybridization of carbon atoms [8](Graf *et al.* 2007). The D band peak is related to the disorder of sp^3 carbon and G peak related to the ordered band of sp^2 bonded carbon atoms. In the Raman spectrum of graphene, peak shift was observed towards the lower region compared to GO. The D and G bands of graphene [9] were observed at 1329 cm^{-1} and 1571 cm^{-1} respectively.

Figure 6 Raman, BET spectra of pure GO



The isotherm of graphene sample as seen in Figure 6 exhibits type II pattern suggesting absence of micro pores. Hysteresis loop type H3 at relatively high pressure suggests presence of asymmetrically slit like pores. The presence of adsorption hysteresis suggests that the isotherm is a pseudo type-II pattern[10]. The type-II isotherm indicates that no micropores or small mesopores exist in the sample. Generally, this kind of behavior is observed due to multilayer adsorption in materials having slit like pores or aggregates of platy particles.

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7. CONCLUSION

In summary, the graphene was successfully synthesized at appropriate temperature via modified hummers method. The XRD spectra show range 10.3 nm conforms the formation of graphene oxide. FESEM micrographs show graphene powder show an agglomerated form with randomly stacked graphene sheets in powder with fluffy like physical appearance and EDS confirms the purity of the samples. The FT-IR results revealed the functional groups of graphene. The Raman analysis confirms the presence of G and D band peaks.

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