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RESEARCH PAPER

Study of the Structural and Electronic Properties of Graphene Nanoribbons with Various Shapes

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ABSTRACT

This study investigates two types of graphene nanoribbons zigzag and armchair analyzing them based on variations in width, length, and edge configuration. For the zigzag type, the widths were set at (4,0) and lengths at 8, 10, and 14 Å. For the armchair type, dimensions of (2,2), (3,3), and (4,4) were used with a length of 6 Å. Electronic and structural properties were calculated using Density Functional Theory (DFT) with the B3LYP functional and the SDD basis set. Geometry optimization was performed, and the absence of imaginary frequencies was confirmed; this ensures the high stability of the studied ribbons, making them suitable for nanotechnology applications. The properties under investigation were calculated using the Gaussian 09 and GaussView5 software packages, following the construction of the structures with Nanotube Modeler. Overall, a decrease in total energy levels was observed across all studied species attributed to the progressive increase in the number of atoms and the consequent variation in HOMO and LUMO energy levels (which determine the material's electronic behavior) along with a reduction in energy gap values. This indicates a correlation between the energy levels and the number of atoms in the structures under study. This theory was employed to analyze the electronic and structural properties of the ribbons; geometric relaxation was performed separately to obtain the geometries required for the study. The density of states (DOS) which determines the number of available electronic states at each energy level within the material was also calculated. Ground-state properties were determined using the time-dependent Schrödinger equation,these calculations encompassed geometric optimization, total energy, molecular orbital energies, the energy gap, infrared (IR) spectra, and ultraviolet-visible (UV-Vis) spectra. Regarding the IR calculations, peaks appeared in the (1450–3000) cm^{-1} wavenumber range for the zigzag type and (950–3200) cm^{-1} range for the armchair type. Furthermore, calculations of ultraviolet and visible spectra revealed a distinct shift in the calculated emission and absorption spectra within the energy ranges of (15.0252–29.0323) eV. and (2.5006–6.3033) eV. between the armchair and zigzag configurations of the studied nanoribbons.

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INTRODUCTION

Graphene is a nanomaterial that consists of one atomic layer of carbon atoms arranged in an ordered two-dimensional hexagonal (honeycomb) lattice. In a graphene sheet, each carbon atom forms three strong covalent σ-bonds with neighboring carbon atoms via sp2 hybridization (an overlap of one s and two p-orbitals) while the unhybridized p-orbital establishes an extended π-bond ("delocalized") system across the surface [1,2]. This unique electronic configuration contributes to graphene exceptional stability and conductivity [3]. Due to its Exceptional carbon-carbon bond strength (∼ 4.9 eV). It is not only mechanically sturdy but also exhibits excellent chemical stability. The monolayer of graphene is impermeable to all gases and liquids [4]. A graphene sheet is cut into finite pieces to form two different edge geometries, zigzag and armchair. Such edges are important to defining the electronic and magnetic properties of material, zigzag edges can harbor localized [5]. Nonbonding edge states with unconventional electronic excitations such excitations can be adjusted by external electric or magnetic fields or through the change of sample geometry. An armchair edge has no such state, but it creates electron wave interference effect in scattering processes.[6]. Graphene has distinctive properties such as ultrahigh electrical conductivity excellent thermal conductivity, superior mechanical strength, large surface area-to volume ratio, and optical transparency make it a highly attractive material for next-generation electronic devices. Among its promised applications, graphene-based sensors for detecting highly toxic gases have attracted growing interest [7].

MATERIALS AND METHODS

The density functional theory with basis sets method is used to calculate the properties of the zigzag and armchair graphene nanoribbons in Fig. 1. The structures of the investigated nanoribbons were designed using the Gaussian View 5.0.8 program [8], and the Austin Model 1 at Gaussian 09 package of programs was initially used to relax the studied structures. For GRNS compounds in their ground state, quantum chemical calculations were carried out. Molecular structures were optimized using Density Functional Theory (DFT) techniques, particularly the popular B3LYP functional, and the SDD basis set to guarantee the accuracy of results regarding molecular geometry optimization and property evaluation [9]. Ground-state energy is included in this study's definition of electronic structure, along with other characteristics like bond energies and molecular orbital energy levels

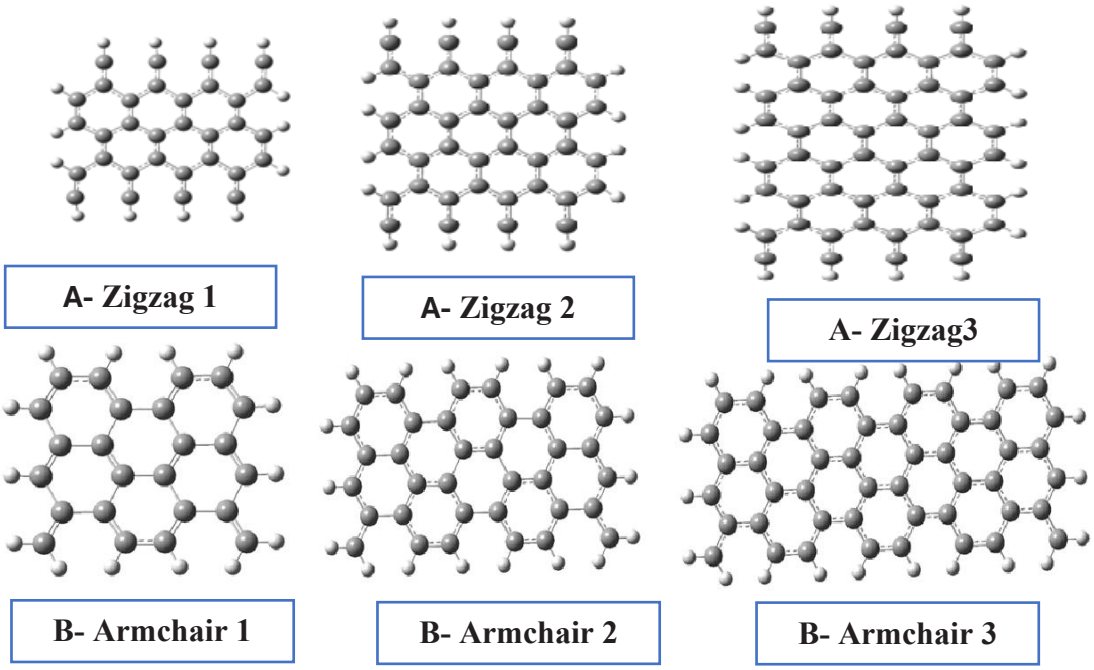

Fig. 1. The geometry optimization for structures graphene nanoribbons (Carbon (C)≡ gray: Hydrogen (H) ≡ white).

(HOMO-LUMO) [10]. Additionally, the Time-Dependent Density Functional Theory (TD-DFT) method was used to analyze the UV-Vis spectrum and infrared (IR) spectra [11].

RESULTS AND DISCUSSION

Computational chemistry programs made use of DFT. As shown in Fig. 1 two types of graphene nanoribbons. The A-zigzag, the first kind, which is composed of three shapes. The B-armchair, the second type, which also comes in three shapes. In order to reduce external influences, hydrogen atoms are bonded to the compound at its outer edges, while carbon atoms are arranged in hexagonal rings in both compounds. Up to the compound's lowest energy, the best geometric optimization was attained. Physicists and chemists consider molecular orbitals and their properties, such as HOMO-LUMO energies, to be especially important parameters in quantum mechanics. Furthermore, the frontier electron density is used to interpret different kinds of reactions in conjugated systems and the most reactive position in Pi-electron systems. The results of conjugate molecules' peripheral interactions are assumed to be the basis for the theory of maintaining orbital symmetry, which depends on the highest occupied molecular orbital (HOMO) or lowest unoccupied molecular orbital (LUMO) for the interacting system. The electronic characteristics of the pure graphene nanoribbons under investigation are shown in Table 1. according to the calculated GNRs energy values for both types, the E_{LUMO} is greater than E_{HOMO}, indicating easy electron transfer through open channels. A mathematical expression for the energy gap is as follows: $E_g = E_{LUMO} - E_{HOMO}$ In armchair GNRs, we find that the energy gap decreases as the number of atoms increase, indicating an increase in ribbon width. This happens because the effect of "quantum

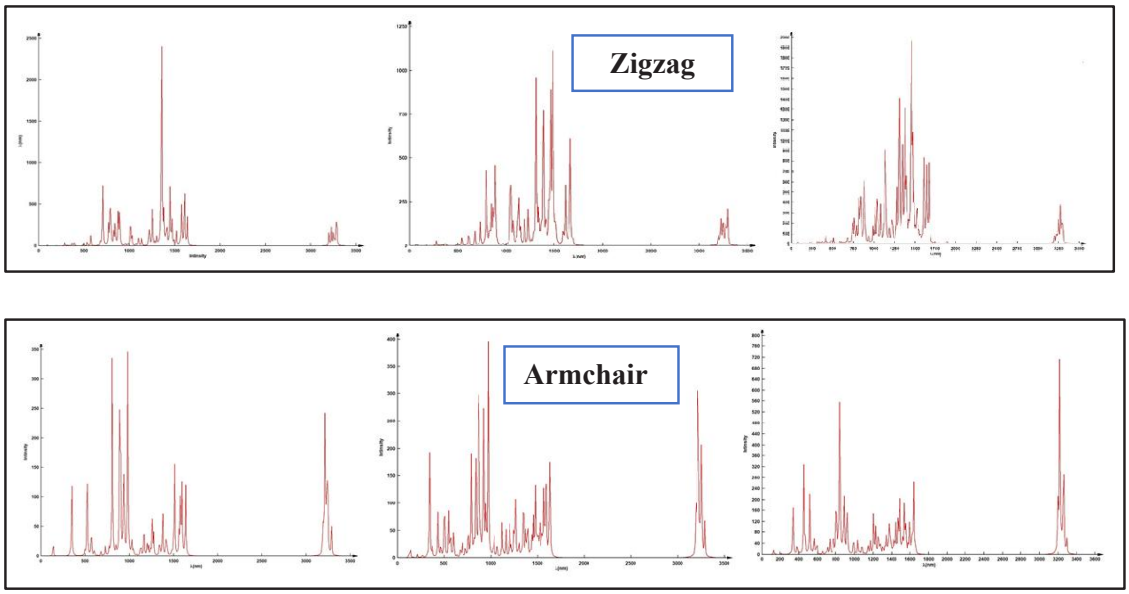

Fig. 2. Shows the zigzag and armchair IR analyses of pure graphene nanoribbons respectively.

Table 1. lists the graphene nanoribbons' electronic characteristics.

Graphene Nanoribbons	E_{HOMO} (eV)	E_{LUMO} (eV)	Eg (eV)	E_T (eV)
Zigzag 1	-4.87791538	-4.40688607	0.47102931	-33404.0707507216
Zigzag 2	-5.36037349	-3.91218283	1.44819066	-41733.4410211636
Zigzag 3	-5.48010364	-3.78537771	1.69472593	-58390.19029554344
Armchair 1	-4.0476956	-3.52795788	0.51973772	-25110.9862007516
Armchair 2	-3.95517684	-3.69013782	0.26503902	-37619.55608400018
Armchair 3	-3.70238295	-3.50809356	0.19428939	-50124.65787817418

confinement" decreases and electrons move more freely as the number of atoms and ribbon width increase. As a result, the energy bands (valence and conduction bands) get closer together, reducing the energy gap.

Conversely, in zigzag GNRs, the energy gap increases with the number of atoms as the edges become farther apart. As the magnetic ordering at each edge becomes more stable and the overlap between them decreases, the energy gap grows. The total energy of graphene nanoribbons decreased as the number of electrons in the sheet increased because the total energy is dependent on the number of electrons in the structure [12].

Infrared spectrum

Normal modes of a simple harmonic oscillator are used to simulate how a molecule vibrates, absorbing and releasing energy. Electromagnetic radiation in the (1–5) × 10^3 cm^{-1}range is known as the infrared (IR) spectrum [13]. For both translation and rotation, the N-atom structure absorbs energy that will oscillate with three degrees of freedom; for vibration, ring molecules will oscillate with (3N-6) degrees of freedom. Fundamental and quasi-fundamental bands are the two types of oscillations in a system. The typical bands are classified as stretch, deformation, wagging, twisting, rolling, and bending oscillations based on high strength and are impacted by additional variations in dipole moments. Non-fundamental bands, and low-intensity hot bands [14]. For pure graphene nano-ribbons, zigzag type showed peaks in the wavenumber range of (1450–3000) cm^{-1}, while the armchair type showed peaks in the range of (950–3200) cm^{-1} (Fig. 2).

UV- Visible radiation

Because matter's energy levels are quantized, only light with a certain energy is absorbed. The range of radiation between 100 and 400 nanometers that is directly below the visible spectrum is known as ultraviolet radiation [15]. Visible or ultraviolet light is absorbed by some molecules. The absorbance of the solution rises with decreasing beam attenuation. The ultraviolet (UV) spectra were calculated using the TD-DFT method with the SDD basis set and the B3LYP hybrid functional. An important step was the calculation of the optical properties of the graphene nanoribbons (their emission and absorption spectra) to determine the shift type (blue or red) and the excitation energy. Emission and absorption spectra of the studied nanoribbons are presented in Fig. 3. It shows how wavelength and absorption are related; the highest absorbance is found at a wavelength of 1200 nm, indicating that a particular electronic transition occurs when a photon with that particular wavelength is absorbed. The number of atoms

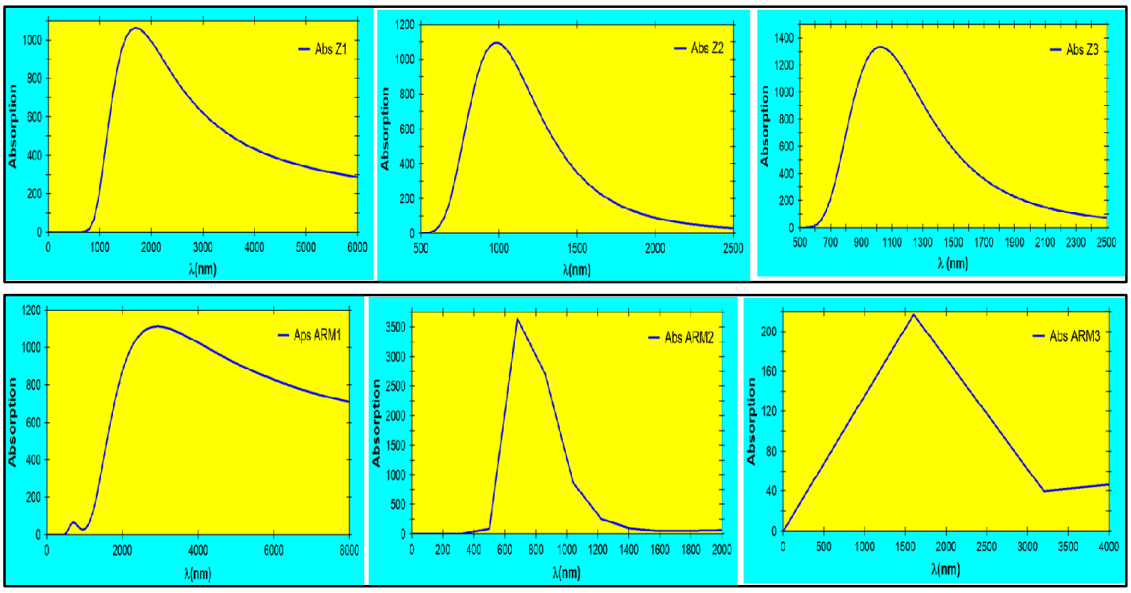

Fig. 3. Displays pure graphene nanoribbons UV-Vis absorption spectra for zigzag and armchair respectively.

in the nanoribbon, and ribbon width, and the edge orientation all affect the oscillator strength at particular wavelengths for the electronic transition peak; the peak rises as the ribbon width and wavelength increase, and vice versa. Because of the symmetry of the structures and the lack of electron scattering centers, the zigzag type results show clarity and regularity. Additionally, it is observed that the absorption peak is located in the ultraviolet spectrum; this is in line with accepted physical principles since wavelength and energy have an inverse relationship.

We observe that the absorption takes place in the zigzag type graphene strips and increases as the wavelength approaches the region of reaction with free electrons.

The transition from the HOMO and LUMO orbit occurs when the energy of the falling photon matches the energy difference between the molecular orbitals. Regarding the type of armchair, we find that the width of the ribbon directly affects the energy gap. These illustrated figures show that the oscillation strength is very high and the peaks in the visible light or infrared region are very clear. The first electronic transition from the top of the valence band to the bottom of the conduction band is represented by the main peak in the above figure, which is followed by a gradual decline. The density of states is responsible for the appearance of the second peak. Generally speaking, we can see from the relationship between absorptivity and wavelength that graphene ribbons only absorb wavelengths with energies equal to the energy difference between the quantized ribbon levels. This explains why the curve abruptly rises at a specific wavelength after starting at zero. From Fig. 4 that emission is more efficient in graphene nanoribbons with an armchair structure than in those with a zigzag structure. This difference is explained by the energy level distribution. The oscillator strength describes how wavelength and emission are related when the ribbon's optical response is 0.02. In these ribbons, the band gap is directly proportional to the width of the ribbon, or more accurately, the number of atoms that comprise the ribbon. High oscillator strength is accompanied by emission regions in both the visible and infrared spectrums. The sharp peaks of these graphene nanoribbons indicate that they act as filters and exhibit strong energy absorption at particular wavelengths.

Density of state

According to quantum mechanics, a system's waves (particles) can occupy particular states and configurations that the system permits, with the system determining the quantized wavelengths [16]. In some systems, the direction of wave propagation is restricted. Because of the crystalline structure of the materials, certain systems only permit wave propagation in one direction. In material physics, a system's DOS is an essential characteristic [17]. The density of states is the number of accessible states per energy unit

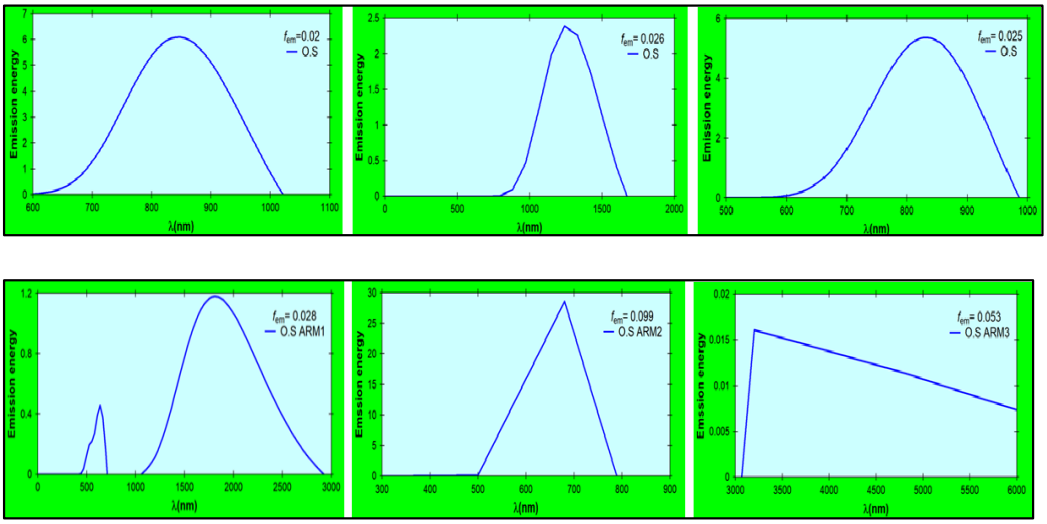

Fig. 4. Displays pure graphene nanoribbons UV-Vis emission spectra for zigzag and armchair respectively.

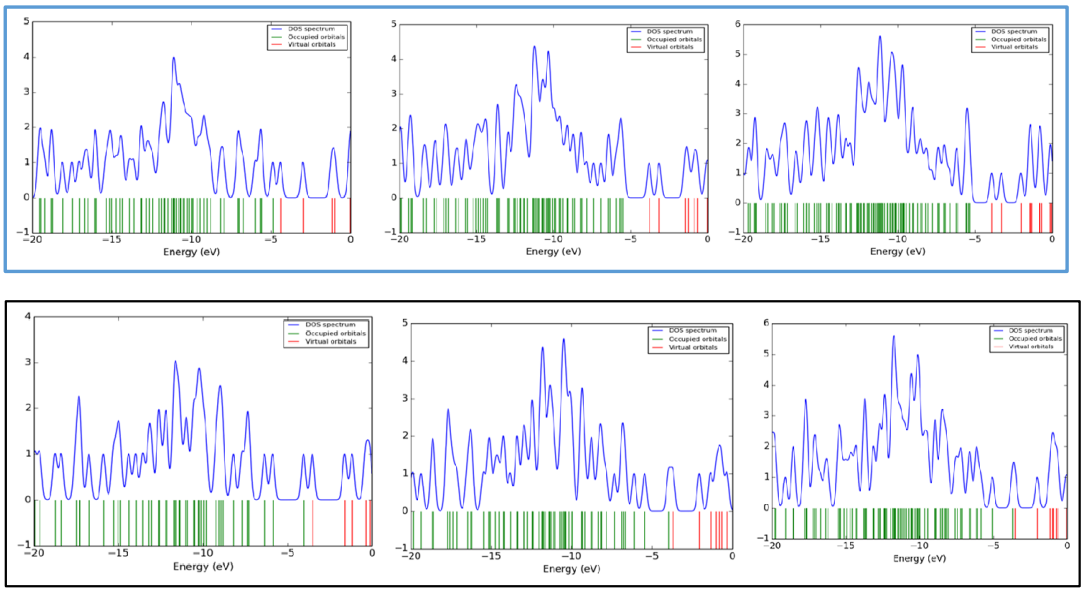

Fig. 5. Shows the DOS of a pure graphene nanoribbons as a function of energy levels for zigzag and armchair respectively.

at each energy level where electron occupation is allowed in the system. The density of states (DOS), or the quantity of orbitals available for each energy level, is represented by the vertical axis . The energy levels, expressed in eV, are displayed on the horizontal axis. Unoccupied orbitals are shown by red lines, whereas occupied orbitals are shown by green lines. The final electron probability, which shows the number of accessible electronic states at each energy, is represented by the blue line and is used to comprehend the electronic behavior of a material. The armchair compound is excellent for gas detection because it has a discernible energy gap, a uniform electron distribution, and is a perfect model for semiconductors. The DOS determines how many states can be occupied at each energy level per energy interval. Fig. 5 shows the DOS of a pure graphene as determined by density functional theory, which is probably caused by local potential fluctuations in the graphene. Pure graphene is highly soluble because only the atomic orbitals of carbon atoms are linearly combined to form molecular orbitals [18].

CONCLUSION

The type of ribbon is largely determined by the total ground-state energy of pristine graphene nanoribbons; for both types of ribbons under study, the total energy decreases linearly as the number of atoms in the ribbon increases. The energy gap (between the LUMO and HOMO orbitals) decreases for one type, according to calculations made using the current theoretical method; this outcome is consistent with experimental data. In contrast, the other type exhibits a slight increase in the energy gap, which is not governed by any particular pattern. Because the atomic orbitals of the carbon atoms combine linearly to form molecular orbitals, pristine graphene nanoribbons have a high solubility. As the wavelength gets closer to the area of reaction with free electrons, the absorption increases in the zigzag-shaped graphene strips. The distribution of energy levels explains why the emission process is more effective in “armchair” graphene nanoribbons than in those with a “zigzag” structure. The band gap in these ribbons is directly proportional to the ribbon width, or more accurately, to the number of atoms that make up the ribbon.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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