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Investigating the Electronic and Optical Characteristics of New Nanocomposites for Flexible Optoelectronics Nanodevices

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This work aims to design of PEO/CuO new structures and investigating optical, and electronic characteristics to use in various electronic and optoelectronics devices like diodes, transistors, photovoltaic cell, electronic gates, sensors and other electronics devices. Using the B3LYP-DFT with a suitable 6-31G basis set for pure PEO and SDD basis set for nanocomposite, a good optimization structure for the predicted nanocomposites was obtained. Geometrical values that have been calculated. The results indicated that the studied nanocomposite need small energy to become cation due to ionization potential is decrease with addition nanoparticle to the pure PEO, but the electronic affinity is an increase with addition nanoparticles to the pure PEO. When compared to other nanocomposite, the total ground state energy of PEO has the highest value of total energy, but ET dropped with the addition of nanoparticles to pure PEO. With the addition of nanoparticles to pure PEO, the hardness decreases, making nanocomposite softer, lowering a species' barrier to losing electrons. The studied nonocomposite direct electronic transition from the valence to conduction band with wave length falls within the solar spectrum range. The results revealed that the (PEO-CuO) nanocomposite has a wide range of applications in the fields of electronics and photo-electronics.

Keywords: electronic devices, optical properties, PEO, energy gap, CuO.

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Introduction

Nanoscience and nanotechnology have gained a lot of attention in recent years. Quantum dots and nanocrystals of metals, semiconductors, oxides, and other materials, as well as one-dimensional nanostructures like nanotubes and nanowires, are important nanoobjects. Synthesis, characterization and applications of these nanomaterials are being explored widely. Single molecule electronics based on nanotubes and nanowires are examples of innovative nanomaterial applications that are emerging, nanocatalysis and biological sensors using nanocrystals or nanotubes. Since the discovery of carbon nanotubes, one-dimensional nanostructures of materials have gotten a lot of attention. Nanotechnology is an essentially interdisciplinary area that has piqued the interest of scientists and engineers in recent years. Nanomaterials can be found all over the world and have been a part of the environment since our planet was formed 4.5 billion years ago[1]. A nanocomposite is a multiphase solid material where one of the phases has one, two or three dimensions of less than 100 nanometers (nm), or structures having nano-scale repeat distances between the different phases that make up the material. In the broadest sense this definition can include porous media, colloids, gels and copolymers, but is more usually taken to mean the solid combination of a bulk matrix and nanodimensional phase(s) differing in properties due to dissimilarities in structure and chemistry. Polymer nanocomposites: Although polymers can be used as structural materials without reinforcement, their usage gets limited due to insufficient mechanical properties. Relatively low strength, coupled with low impact strength, is a characterization of polymer materials. Polymer nanocomposites represent a new alternative to conventionally filled polymers. Polymer Nanocomposites are materials in which nanoscopic inorganic particles, typically 10-100 Å in at least one dimension, are dispersed in an organic polymer matrix such as polyacetylene, polythiophene, and polypyrrole. Because of their nanometer sizes of the inorganic filler Nanocomposites exhibit markedly improved properties when compared to the pure polymers or their traditional composites [2]. One of the few biodegradable synthetic polymers approved for internal usage in cosmetics, foods, pharmaceuticals, and personal care products, is polyethylene oxide (PEO). PEO is an efficient polymer conductive ion [3]. PEO can be categorized as a semi-crystalline polymer resulting from partial regularity of its structure. PEO is a linear enteric polymer that dissolved in various types of inorganic salts even at very high concentrations, where the ether oxygen atoms(-Ö-) throughout the backbone of PEO are closely involved in the complexation of metal salt cations [4]. Also, the flexible formation of C–O–C stretching in the backbone of the PEO chain gives the material with excellent toughness [5]. CuO has attracted much attention. CuO is a p-type semiconductor material with small band gap energy of only 1.2 eV at room temperature. It has been shown that CuO can be used in high temperature high temperature superconductors, gas sensor, magnetic storage media, catalysis and field emitters. The nanocomposites have different applications in many fields such as pressure sensor antibacterial and energy storage [6]. The present work aims to design of PEO/CuO composites and investigating their optical, electronic properties for nanosemiconductors devices with lightweight and few cost.

I. Theoretical Part

The density functional theory (DFT) is a one-spin density functional theory. There are three spatial coordinates for each electron (assuming fixed). Nuclear sites) is not intuitive in and of itself for systems with more than one electron. One may, in fact, approach the Hartree–Fock HF approximation in the same way you would the Hartree–Fock HF approximation. A philosophical instrument rather than a mathematical one. By allowing the wave function to be expressed as a Slater determinant of one-electron orbitals, the chemist gains some clarity by being able to describe each electron separately, believed to be loosely self-contained [7-11].

Because a total energy of system is the sum of its kinetic and potential energy, the total energy of molecule must be at its lowest at the optimal shape. When a molecule reaches equilibrium, it is said to be in a balanced condition. The resultant of the effective forces is zero [12].

The ionization energy of a chemical species is the minimum energy necessary to remove an electron from a gaseous atom in its ground state (an atom or molecule). The ionization energy of large atoms or molecules is low, whereas the ionization energy of small molecules is high. Ionization energies are generally higher [13-15]:

$$Energy + X(g) \rightarrow X^{+}(g) + e^{-}, \qquad (1)$$

where X represents an atom.

When one electron is added to a neutral atom or molecule to generate a negative ion, the E_A of the atom or molecule is defined as the amount of energy released [16-17]:

$$X(g) + e^{-} \rightarrow X^{-}(g) \qquad (2)$$

The difference between the total energies for the ground state of a molecule and the ground state of the relevant ion can be used to calculate the E_A and I_E. Differences in energies obtained using correlated quantum mechanical approaches yielded extremely accurate results, often more accurate than might be obtained by experimental methods [18]. The ionization potential is calculated in present work as the energy difference between the energy of the molecule derived from electron-transfer (radical cation) and the respective neutral molecule [19-24]

$$I_E = E_{cation} - E_n \qquad (3)$$

The E_A was calculated as the difference in energy between the neutral and anion molecule:

$$E_A = E_n - E_{anion} \qquad (4)$$

In the scope of Koopmans theorem, the HOMO and LUMO energy were also employed to estimate the I_E and E_A. [7-9,25-28]

$$I_E = -HOMO \qquad (5)$$

$$E_A = -LUMO \qquad (6)$$

The hardness H is a measurement of molecule resistance to the change or deformation. defined as [10-15]:

$$H = \frac{1}{2}\left[\frac{\delta\mu}{\delta N}\right] V(\vec{r}) \qquad (7)$$

In terms of ionization potentials I_E and electron affinities E_A, the hardness is half of the energy gap between two frontier orbitals [16-20]:

$$H = \frac{I_E - E_A}{2} \qquad (8)$$

A solid molecule has a large energy gap. The theoretical definition of chemical hardness was provided by DFT as the second derivative of electronic energy with respect to the number of electrons N, for a constant external potential $V(\vec{r})$ [21]

$$H = \frac{1}{2}\left[\frac{\delta^2\mu}{\delta^2 N}\right] V(\vec{r}) \qquad (9)$$

$$S = \frac{1}{2H} = \left[\frac{\delta^2\mu}{\delta E^2}\right] V(\vec{r}) = \left[\frac{\delta N}{\delta\mu}\right] V(\vec{r}) \qquad (10)$$

The energy gap in the soft molecule is minimal. Soft molecules will be more reactive than hard molecules because they have a smaller energy gap, which means lower excitation energies for the manifold of excited states. Their electron density changes more easily than a hard molecule, and as a result, soft molecules will be more reactive than hard molecules [22].

Changes in the electron density of a system are caused by the mixing of suitable excited state wave functions with the ground state wave function in quantum theory. The electronegativity is defined as the negative of the chemical potential in DFT and is a measure of an atom's tendency to attract electrons in a chemical bond [25,29-31]:

$$\chi = -\frac{I_E + E_A}{2} \qquad (11)$$

where χ is electronegativity. The electrophilicity index is a measure of energy lowering due to maximal electron flow between donor and acceptor. Electrophilicity index [32-35] is defined as:

$$W = \frac{K^2}{2H} \tag{12}$$

II. Results and Discussion

Many of a molecule's physical and chemical properties are determined by its optimal structure. It is required to determine the molecule's relaxation, in which the optimum structure is the structure with the least amount of energy. The relaxed structures of pure (PEO) and (PEO-CuO) nanocomposite in the gas state were derived using the DFT approach with Becke's three-parameter hybrid functional (B3LYP) and 6-31G and SDD basis sets for PEO and nanocomposite, respectively, these procedures are shown in Figs. 1 and 2. Table 1 shows the geometric parameters of (PEO) and (PEO-CuO). The calculated values of bonds in this work agreement with the studies [36-40]. Figures 3 and 4 show the results of FTIR of (PEO) and (PEO-Cu) structure. The FTIR results of structure illustration the (CuO) interactions with (PEO) which include different in an intensities and the shift in several bonds.

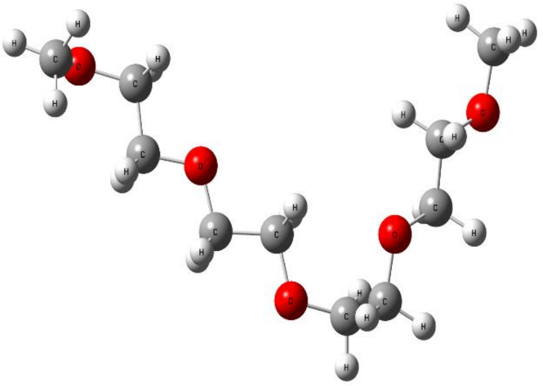

Fig. 1. The relax structure of (PEO) by DFT-B3LYP/6-31G.

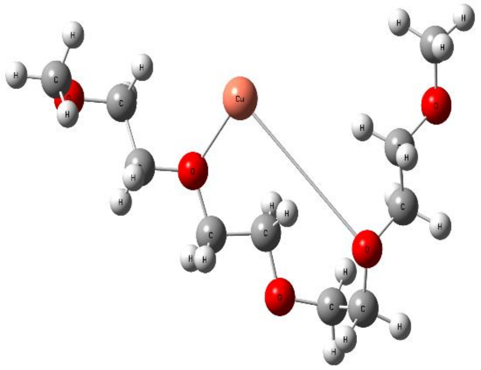

Fig. 2. The relax structure of (PEO–CuO) nanocomposite by DFT-B3LYP/SDD.

Density functional theory (DFT) has been used to compute the electronic properties, like energy gap, (E_{HOMO}), (E_{LUMO}), total energy, I_E, E_A, X, H, S, W.

The Density Functional Theory, at the B3LYP level with 6-31G basis functions for PEO and the SDD basis for the nanocomposite are used. To clarification and understanding the performance of the absorption spectra of the pure PEO and nanocomposite, it is necessary to studying the electronic structures for the studied nanocomposites.

Table 1

Average lengths of bond in (Å) and the angles in degree.

Measurements	Optimization parameters	Values
Bonds, Å	(C-C)	1.53602
	(C-O)	1.45968
	(C-H)	1.09587
	(Cu-O)	2.14762
	(O-Cu)	4.77408
Angles, deg.	(C-O-Cu)	120.85362
	(H-C-C)	110.168
	(H-C-O)	110.573
	(O-C-H)	109.58210
	(H-C-H)	109.39855
	(C-C-H)	111.57057

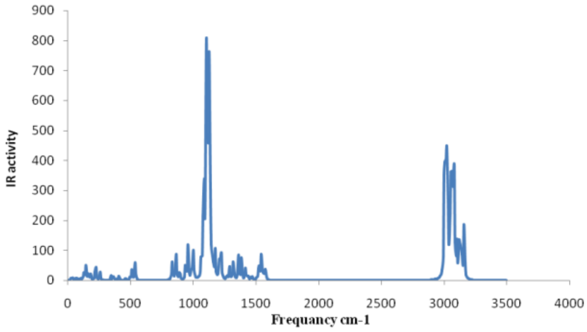

Fig. 3. IR spectrum of (PEO) at the B3LYP/ 6-31G basis set.

Figures 5 and 6 shows the UV-Vis spectra Visible and Ultra Violet spectrum is reliant on upon the electronics structure of the molecule. From Figs. 5 and 6, absorption intensity of (PEO-CuO) have higher UV-Vis spectra. As a result, it shows that absorption increases with increasing the number of atoms, this is owing to the moving electrons from valance level to the conduction band at these energies, hence increase in absorption due to the increase in a number of charges carriers [41-44].

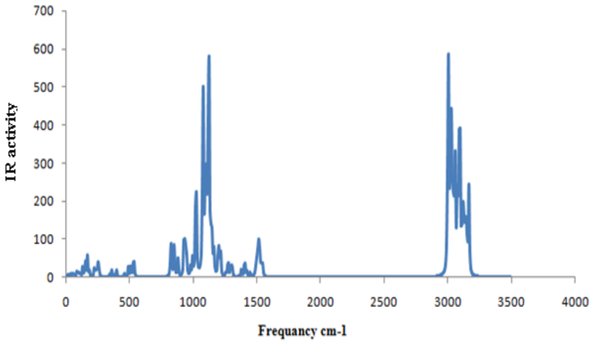

Fig. 4. IR spectrum of(PEO-CuO) at the B3LYP/ SDD basis set.

Density functional theory (DFT) has been used to compute the electronic properties, like energy gap, (E_{HOMO}), (E_{LUMO}), total energy, I_E, E_A, X, H, S, W. The Density Functional Theory, at the B3LYP level with 6-31G basis functions for PEO and the SDD basis for the nanocomposite are used. To clarification and understanding the performance of the absorption spectra of the PEO and nanocomposite, it is necessary to studying the electronic structures for the studied nanocomposites.

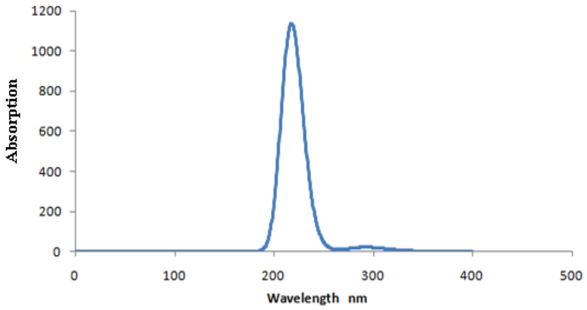

Fig. 5. UV-Vis spectrum for (PEO) using B3LYP/ 6-31G.

Table 2 shows the calculated frontier molecular orbitals (FMOs) energies (High Occupied Molecular Orbital HOMO and Low Unoccupied Molecular Orbital LUMO) and LUMO–HOMO energy gap *Eg* of each nanocomposite. The consequences in Table 2 observed that the energies of HOMO and LUMO of the studied nanocomposite are changed expressively. The consequences showed the HOMO and LUMO are slightly different and this suggests that different structures pay significant roles on electronic properties and improving the electron accepting ability and the effect of symmetry and distribution nanocomposite on the energies of HOMO and LUMO cannot be ignored [45]. The consequences showed the presence of the electron attracting CuO nanoparticle in the molecule. leads to lowering the LUMO and therefore reducing the energy gap.

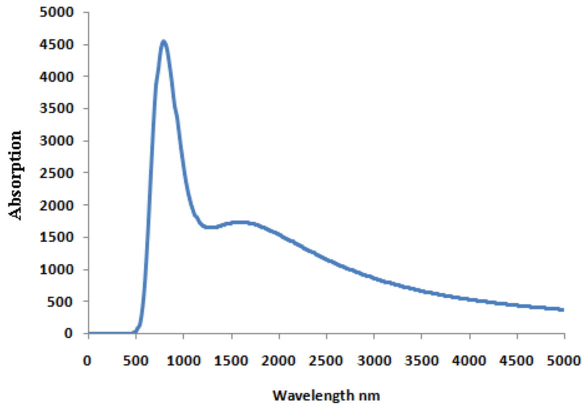

Fig. 6. UV-Vis spectrum for (PEO-CuO) using B3LYP/ SDD.

The energy gap *Eg* for the studied nanocomposite was obtained from the separation LUMO–HOMO energy by using the B3LYP/(6-31G basis set for pure PEO and SDD basis set for (PEO-CuO nanocomposite)-DFT calculations. The calculated energy gaps were decreased in the following order [46]:
(PEO-CuO) (3.8036 eV) < (PEO) (8.1398 eV).
As noticed, the energy gap of pure PEO molecule decreases with the addition of CuO nanoparticle. The change of the $_{Eg}$ of the structure is because of the changes in both HOMO and LUMO energies, and constructed the molecular orbitals according to the linear combination of atomic orbitals LCAOs.

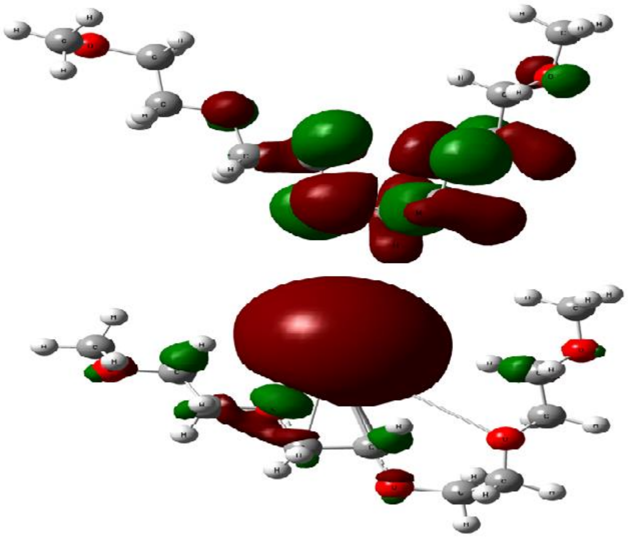

Fig. 7. The distribution of HOMO (up) and LUMO (down) for (PEO).

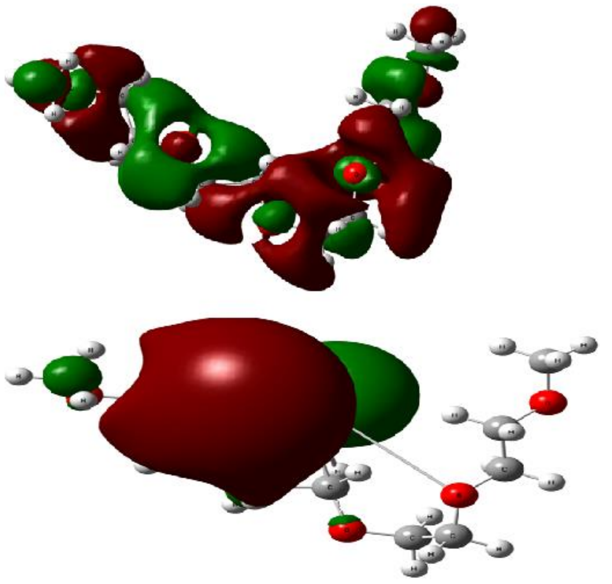

Fig. 8. The distribution of HOMO (up) and LUMO (down) for (PEO-CuO).

The values of the ionization potential IE and electron affinity E_A determined using Koopmans Theorem (KT) for the structures under investigation are shown in Table 2. In comparison to the reference molecule pure PEO, the nanocomposite has low I_E and high E_A values. The pure PEO's I_E was reduced while the E_A was raised after the nanoparticle was added. In comparison to pure PEO, (PEO–CuO) nanocomposite has the smallest value of IE, which suggests that (PEO–CuO) nanocomposite requires less energy to become a cation or anion [47-49].

$$E_{tot} \approx E_{tot}\left(PEO\right) + n \cdot E_{tot}\left(N\right) \tag{13}$$

where E_{tot} (PEO) =− 770.105 in (a.u.), n is the number of addition nanoparticles.

Table 3 shows that PEO has the highest total energy

Table 2

Some electronic properties for pure PEO and nanocomposite from DFT-B3LYP/SDD basis set.

PEO					PEO-CuO				
E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	I_E (eV)	E_A (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	I_E (eV)	E_A (eV)
-6.4811	1.6587	8.1398	6.4811	-1.6587	-3.9857	-0.182	3.8036	3.9857	0.182

Table 3

The calculated energies ET, χ, H, S and ω for pure PEO and nanocomposite DFT-B3LYP/6-31G and SDD basis set.

PEO					PEO-CuO				
E_T a.u.(eV)	χ(eV)	H(eV)	S(eV)	ω(eV)	E_T a.u. (eV)	χ (eV)	H(eV)	S(eV)	ω (eV)
-770.105	-2.4112	4.0699	0.1228	0.7142	-967.58	-2.0838	3.8037	0.1314	0.5707

value when compared to other nanocomposite materials, with the addition of nanoparticles to pure PEO, ET dropped. This result reflects each structure's binding energy and demonstrates that these structures have good relaxation. This leads to be certain that the effect of adding CuO atoms in pure PEO on the total energy of the molecule is effective [50, 51]. Table 3 shows that when compared to pure PEO, the electrochemical hardness H of (PEO-CuO) nanocomposite has the lowest values and the highest electronic softness S. The primary future indicators are low H and high S, indicating that the band gap will be rather soft. These findings are consistent with the energy gap that the structures have, and they point to the pure PEO's high activity in response with the surrounding species [52]. Also the calculated values of the electronegativity χ of pure PEO and nanocomposite. As shown, the maximum value of χ is (-2.0838) eV for (PEO–CuO) nanocomposite and the minimum value is (-2.4112) eV for (PEO) nanocomposite. This result is because of the difference of the configuration of the nanocomposite under study.

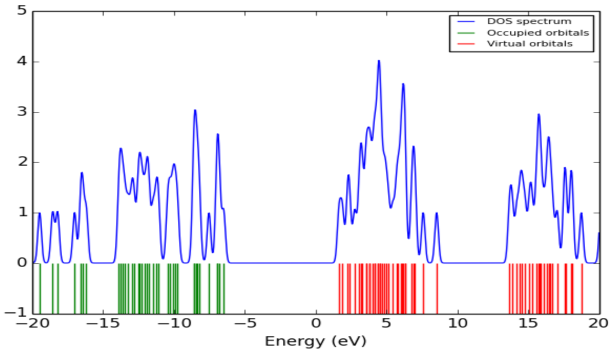

Fig. 9. DOS of (PEO) structure.

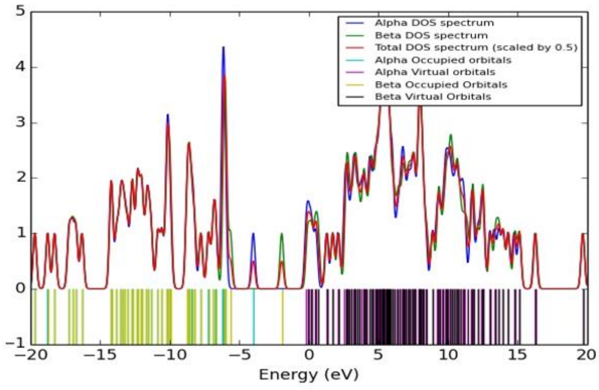

Fig.10. DOS of (PEO-CuO) structures.

The great electronegativity of nanocomposite allowed it to donate and accept electrons from the surrounding species [53]. Table 3 declares the electrophilicity for pure PEO and nanocomposite. The contribution of the frontier molecular orbitals FMOs to determining the charge separated states of the nanocomposite under study comes from these values. Figures 7 and 8 show the electronic structures of the HOMO and LUMO of pure PEO and nanocomposite. As shown, because of the linear combination of atomic orbitals and molecular orbitals, the presence of CuO nanoparticles in the structure of pure PEO affects the map of HOMO and LUMO distribution, changing the molecule's symmetrical point group [54-56].

As shown in Figures 9 and 10, the density of states of (PEO) and (PEO-CuO) structures with energy levels were computed using the DFT-B3LYP/SDD level of theory. For pure, the charge density is low in occupied orbitals and high in virtual orbitals in the density of states (DOS) spectrum. The (PEO-CuO) nanocomposite is in a doublet state, whereas the other nanocomposite is in a singlet state. The degeneracies of vacant molecular orbitals are greater than those of occupied molecular orbitals in these circumstances. Hybridization of OPEO and Cu orbitals forms the majority of the bonds.

Conclusions

Design of novel PEO/CuO structures for usage in modern electrical and optoelectronic devices is part of the current work. Structure, optical, and electrical properties have all been studied. Using the B3LYP-DFT and an appropriate 6-31G and SDD basis set for pure PEO and nanocomposite, a good optimization structure for the predicted nanocomposites was obtained. Geometrical values that have been calculated. The nanocomposites' parameters are in good accord. Due to the presence of both HOMO and NMOS, they are the closest to semiconductors and LUMO levels become more closely related. All the studied nanocomposite need small energy to become cation due to ionization potential is decrease with addition nanoparticle to the pure PEO, but the electronic affinity is an increase with addition nanoparticles to the pure PEO. When compared to other nanocomposite, the total ground state energy of PEO has the highest value of total energy, but ET dropped with the addition of nanoparticles to pure PEO. With the addition of nanoparticles to pure PEO, the hardness decreases, making nanocomposite softer, lowering a species' barrier to losing electrons. The wavelength of the analyzed nonocomposite direct electronic transition from the valence to conduction band falls within the solar spectrum region. The (PEO-CuO) nanocomposite offers a wide range of applications in the disciplines of electronics and photo-electronics, according to the findings.

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Дослідження електронних та оптичних характеристик нових нанокомпозитів для гнучких нанопристроїв оптоелектроніки

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Робота спрямована на розробку нових структур PEO/CuO та дослідження їх оптичних та електронних характеристик для використання в різних електронних та оптоелектронних пристроях, таких як діоди, транзистори, фотоелектричні елементи, датчики та інші електронні пристрої. Використовуючи B3LYP-DFT з відповідним базовим набором 6-31G для чистого PEO та базовим набором SDD для нанокомпозиту, отримано хорошу оптимізаційну структуру для прогнозованих нанокомпозитів. Розраховано геометричні параметри. Результати показали, що досліджуваному нанокомпозиту потрібна невелика енергія, щоб стати катіоном, оскільки потенціал іонізації зменшується з додаванням наночастинок до чистого PEO, при цьому електронна спорідненість збільшується із додаванням наночастинок до чистого PEO. У порівнянні з іншими нанокомпозитами, загальна енергія основного стану PEO володіє найвищим значенням повної енергії, але ET падає при додаванні наночастинок до чистого PEO. З додаванням наночастинок до чистого PEO твердість зменшується, роблячи нанокомпозит м’якшим, знижуючи бар’єр для втрати електронів. Досліджуваний нанокомпозит характеризується прямим електронним переходом із валентної зони в зону провідності із зменшенням довжини хвилі в межах сонячного спектру. Результати показали, що нанокомпозит (PEO-CuO) має широкий спектр застосування в галузях електроніки та фотоелектроніки.

Ключові слова: електронні пристрої, оптичні властивості, PEO, заборонена зона, CuO.