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Exploring the Structure, Optical and Electronic Properties of New PVA–PEO–Ba–Si_3N_4 Structures for Electronics Applications

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The present work aims to design the new PVA–PEO–Ba–Si_3N_4 structures to use them in various optoelectronics nanodevices. The structural, thermal, optical and electronic characteristics of PVA–PEO–Ba–Si_3N_4 structures are studied. The structure of PVA–PEO–Ba–Si_3N_4 is analysed by GaussView 5.0.8 and relaxed using the Gaussian 09 package of programs employing the density functional theory (DFT) with the B3LYP/LanL2DZ level. The studied characteristics of PVA–PEO–Ba–Si_3N_4 structures include the energy, ionization potentials, energy gap, and electron affinity. The PVA–PEO–Ba-Si_3N_4 structures are optimized successfully with the Gaussian 09 package. The results show that the PVA–PEO–Ba–Si_3N_4 structures have good optical and electronic properties. In addition, the PVA–PEO–Ba–Si_3N_4 nanostructures have wide absorption spectrum that makes the PVA–PEO–Ba–Si_3N_4 structures suitable in various electronics devices like transistors, photovoltaic cell, sensors and other devices.

Цю роботу спрямовано на розробку нових структур полівініловий спирт (ПВС)–поліоксиетилен (ПОЕ)–Ba–Si_3N_4 для використання в різних нанопристроях оптоелектроніки. Досліджено структуру, теплові, оптичні й електронні характеристики структур ПВС–ПОЕ–Ba–Si_3N_4. Структуру ПВС–ПОЕ–Ba–Si_3N_4 було проаналізовано за допомогою GaussView 5.0.8 і зрелаксовано за допомогою пакета програм Gaussian 09, що використовує теорію функціоналу густини (DFT) на рівні B3LYP/LanL2DZ. Досліджувані характеристики структур ПВС–ПОЕ–Ba–Si_3N_4 включали енергію, потенціяли йонізації, енергетичну щілину та спорідненість до електрона. Структури ПВС–ПОЕ–Ba–Si_3N_4 були успішно оптимізовані за допомогою пакета Gaussian 09. Результати показали, що структури ПВС–ПОЕ–Ba–Si_3N_4 мають хороші оптичні й електронні властивості. Крім того, наноструктури ПВС–ПОЕ–Ba–Si_3N_4 мають широкий спектер поглинання, що робить структури ПВС–ПОЕ–Ba–Si_3N_4 придатними для різних електронних пристроїв, таких як транзистори, фотоелектричні елементи, давачі й інші пристрої.

Key words: polymer blend, Si_3N_4, optical properties, Gaussian 09, electronics devices.

Ключові слова: полімерна суміш, Si_3N_4, оптичні властивості, Gaussian 09, електронні пристрої.

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1. INTRODUCTION

Polymers are considered as organic materials, which have conjugated chains and show high electrical conduction; this one relates to their characteristics such charges' carriers as *p*-electrons, which cause the mobility of charge alongside the polymers' chain backbone as well, inorganic materials like metal oxides and metals. Polymers' characteristics are as good as with inorganic materials although polymers have some pros and cons, like flexibility, low cost, processability, lightweight, and resistance to corrosion. The inorganic materials as well have important characteristics like good mechanical strength and high thermal stability. Thus, polymer/inorganic systems have different applications in various fields [1]. The improvement of practical organic materials is a quickly increasing of science area, which possibly may replace the conventionally employed materials with low cost and improved performing novel ones in the future and carry out several novel applications [2, 3]. The Si_3N_4 material has large chemical stability, resistance to heat and mechanical characteristics [4]. Gaussian 03 program (computer software is to make the calculation, which is capable of predicting various characteristics of reactions and molecules, including the structures and molecular energy [5]. There are numerous studies on composites and nanocomposites to utilize in a variety of fields like antibacterial defence [6–12], electronics and optoelectronics [13, 30], energy storage [31–33], radiation shielding and bioenvironmental technology [34–39], optical fields [40–51] and sensors [52, 53]. The present work aims to design of novel PVA–PEO–Ba–Si_3N_4 structures for flexible optoelectronics devices. The PVA/PEO blend doped with barium and Si_3N_4 have promising materials in the flexible and low-cost applications for different modern industrial fields.

2. THEORETICAL PART

Energy gap (E_g) is the difference between the energies of (HOMO) and (LUMO) [5]:

$$E_{gap} = E_{LUMO} - E_{HOMO}. \tag{1}$$

The ionization energy is expressed (in [eV]) by [54] as follows:

$$I_E = -E_{HOMO}. \tag{2}$$

Electron affinity can be defined by [5] as follows:

$$E_A = -E_{LUMO}. \tag{3}$$

The chemical potential (μ) is determined by [55] as follows:

$$\mu \approx \frac{1}{2}\left(E_{HOMO} + E_{LUMO}\right) \approx -\frac{1}{2}\left(I_E + E_A\right). \tag{4}$$

Chemical hardness (H) is given by [56] as follows:

$$H = \frac{I_E - E_A}{2}, \tag{5}$$

Chemical softness (S) is the inverse of hardness by [57] as below:

$$S = \frac{1}{2H}, \tag{6}$$

Electrophilicity (ω) can be defined by [58] as follows:

$$\omega = \frac{\mu^2}{2H}. \tag{7}$$

The electronegativity (E_N) is given by [59] as follows:

$$E_N = \frac{1}{2}\left(I_E + E_A\right). \tag{8}$$

The electric dipole polarizability represents a second order variation in energy [60]. The polarizability is given by [61] as follows:

$$\langle\alpha\rangle = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right). \tag{9}$$

4. RESULTS AND DISCUSSION

The structure of PVA–PEO–Ba–Si_3N_4 was designed by GaussView 5.0.8 and relaxed using the Gaussian 09 package of programs by employing the DFT with the B3LYP/LanL2DZ level. Figure 1 shows the optimized relaxed PVA–PEO–Ba–Si_3N_4 structure. Table 1 represents the standard orientation of all atoms in the molecule. The

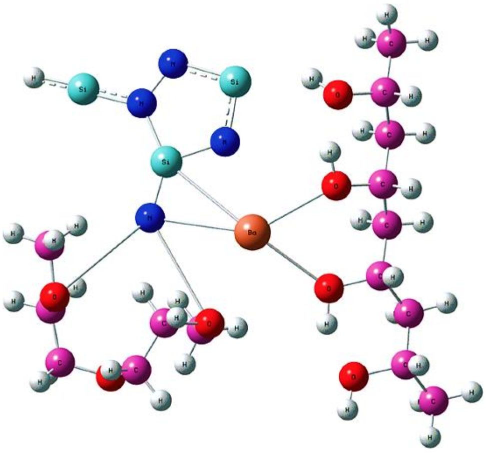

Fig. 1. Optimization of PVA–PEO–Ba–Si_3N_4 structure.

TABLE 1. Average lengths of bond in [Å] and the angles in [degrees].

Measurements	The optimization parameters	Values
Bonds, Å	C–C	1.532
	C–O	1.481
	C–H	1.099
	O–H	0.993
	Si=N	1.755
	N–N	1.411
	Ba–Si	3.271
Angles, deg.	C–C–C	113.201
	C–O–H	106.959
	N–Si–N	121.899
	Ba–N–Si	152.830

bonds' values in present work are agreed with Refs. [4, 62, 63].

Figure 2 shows the IR spectrum of PVA–PEO–Ba–Si_3N_4 structure calculated using DFT. As found, the strong peak observed at 3300 cm^{-1} is attributed to the O–H groups.

In the Raman spectra, a variation is observed in the molecules' polarization; that is, the ultraviolet or visible photons interact with the vibrating bonds of molecules losing or gaining parts of their energy, thereby, creating the spectra [64]. Figure 3 represents the Raman spectra of PVA–PEO–Ba–Si_3N_4 structure. Intensities of Raman spectra depend on the probability that photon with particular wavelength will be absorbed. As seen in figure, the active IR

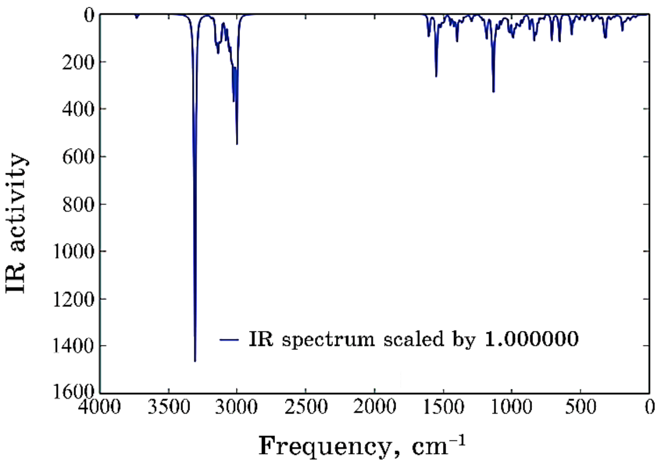

Fig. 2. IR spectra of PVA–PEO–Ba–Si_3N_4 structure.

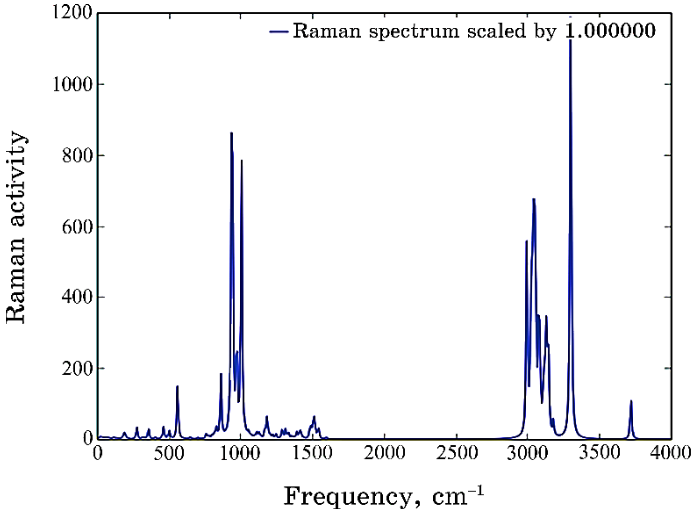

Fig. 3. Raman intensities of PVA–PEO–Ba–Si_3N_4 structure with vibration frequency.

region is similar with less activity in Raman intensities. The peak intensities in Raman spectrum depend on the probability that a particular wavelength photon will be absorbed. These probabilities can be computed from the wave function by computing the transition dipole moments. This gives relative peak intensities, since the calculation does not include the density of the substance.

The time dependence of electron absorption spectra of PVA–PEO–Ba–Si_3N_4 was performed using TD-SCF at B3LYP/DFT level of calculations.

Figure 4 show the visible and ultraviolet spectra. The UV-Vis-calculations of PVA–PEO–Ba–Si_3N_4 composites carried out by means of the B3LYP-TD/6-31G method included the excitation energy, wavelength, oscillator strength and electronic transition. The spectrum lies within the UV-Vis limits, because the spectrum in theoretical study taking into account concentrations will be calculated at the highest concentration, where the sample will be completely opaque only seen in the visible area of the spectrum, and, at the lower concentration, it will be seen in the ultraviolet area of the spectrum.

The NMR data of PVA–PEO–Ba–Si_3N_4 composites are given in

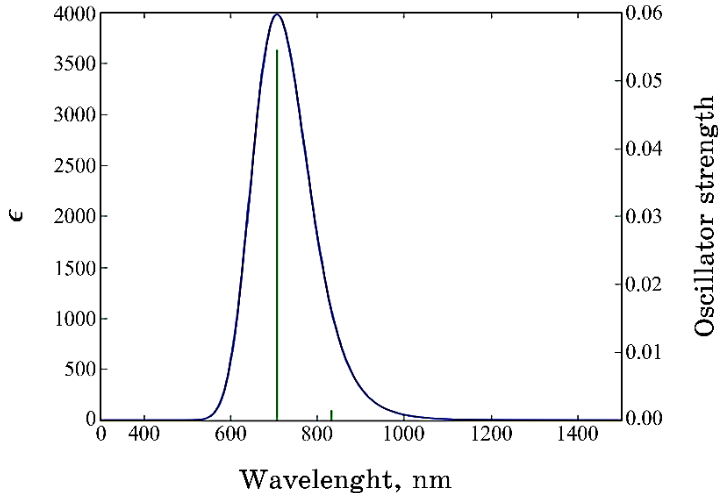

Fig. 4. UV-Vis spectrum for PVA–PEO–Ba–Si_3N_4 structures.

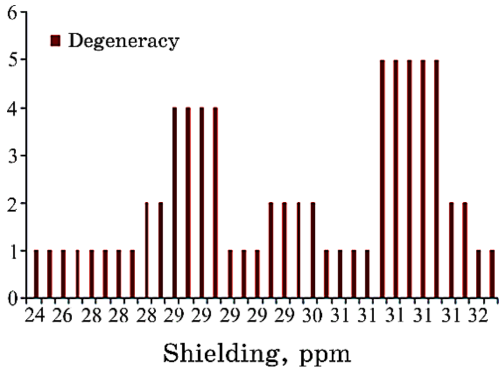

Fig. 5. Nuclear magnetic resonance of PVA–PEO–Ba–Si_3N_4 structures.

Fig. 5. ^{1}H-NMR reveals several types of protons in high shielding. The high shielding of H may be resonated to the H-bond formation with N and O atoms in ammine and hydroxyl ligands.

Table 2 gives the values of E_{HOMO}, E_{LUMO} and E_g in [eV] for PVA–PEO–Ba–Si_3N_4 structure. The E_{LUMO} is larger than the E_{HOMO} with big separation between the two molecular orbitals ($E_g = 5.75$ eV). This behaviour is in a good agreement with Refs. [4, 65] and refers that PVA–PEO–Ba–Si_3N_4 structure requests high energy to accepting or donating an electron. Concerning DOS spectra, the charge density is small in occupied orbital and elevated in virtual orbital for pure, O- and H-substituted Si_3N_4 structures. This mentions the localization of charges along the virtual orbitals rather than in occupied orbitals.

Figure 6 shows the LUMO and HOMO distributions for PVA–PEO–Ba–Si_3N_4 structures.

Figure 7 represents the electrostatic potential (ESP) distribution

TABLE 2. Energy gap values in [eV] for structures.

PVA–PEO–Ba–Si_3N_4 structures		
E_{HOMO}, eV	E_{LUMO}, eV	E_g, eV
–9.01	–3.26	5.75

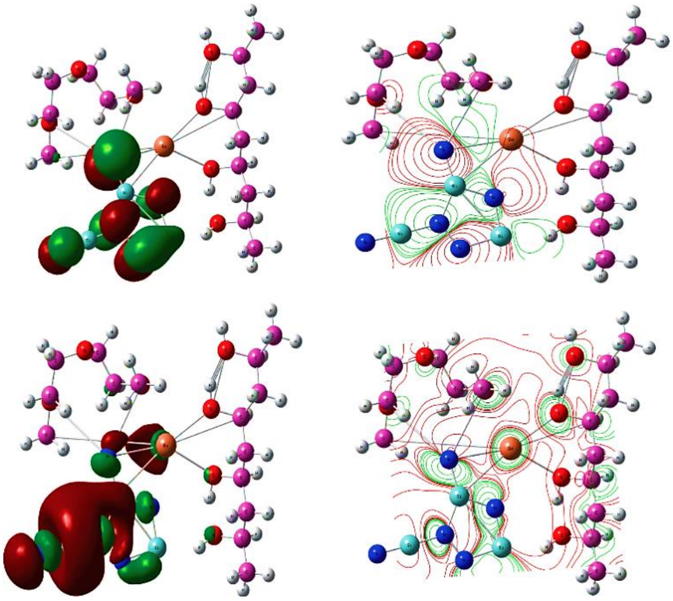

Fig. 6. The distribution of HOMO(up) and LUMO(down) for PVA–PEO–Ba–Si_3N_4 structures.

for PVA–PEO–Ba–Si_3N_4 structures from the total self-consistent field (SCF) approximation. ESP distributions for PVA–PEO–Ba–Si_3N_4 structures are created by repulsive forces or attracting regions around each structure. In commonly, the ESP surfaces for PVA–PEO–Ba–Si_3N_4 structures are dragged toward the positions of negative charges in each molecule based on the high electronegativity oxygen atoms (3.5 eV).

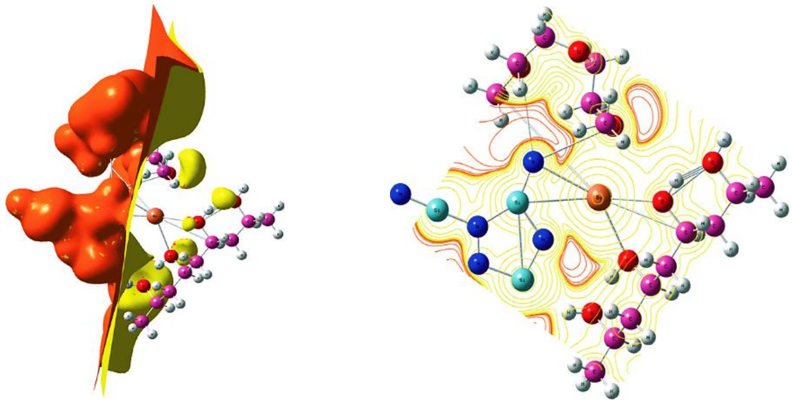

Fig. 7. Electrostatic-potential distribution surface for PVA–PEO–Ba–Si_3N_4.

TABLE 3. Electronic-characteristics values in [eV] for the structures.

Property	PVA–PEO–Ba–Si_3N_4 composites
Total energy	–1428.997 (a.u.)
Ionization potential	9.01
Electron affinity	3.26
Electronegativity	6.135
Chemical hardness	2.875
Chemical softness	0.173
Chemical potential	–6.135
Electrophilicity	6.545
Dipole moment [Debye]	27.149

TABLE 4. The calculated average $\langle\alpha\rangle$ and its components for PVA–PEO–Ba–Si_3N_4 composites.

Polarizability, a.u.			
α_{xx}, a.u.	α_{yy}, a.u.	α_{zz}, a.u.	$\langle\alpha\rangle$, a.u.
409.985	402.077	234.338	348.8

Table 3 represents the ground state energy (E_T) results in [a.u.]. These characteristics include I_E, E_A, E_N, H and ω [66].

Table 4 shows the average polarizability ⟨α⟩ and its components in [a.u.] for PVA–PEO–Ba–Si_3N_4 structures.

The density of states (DOS) for PVA–PEO–Ba–Si_3N_4 structures as a function of energy levels was calculated by the DFT-B3LYP/LanL2DZ level of theory. Figure 8 shows the degenerated states as a function of energy levels for the structure; this degeneracy is caused by the existence of the new types of atoms that leads to varying the bond lengths and angles or changing the geometry of the structure.

Table 5 represents the E_{th}, C_v and S_{th} values of thermal characteristics for PVA–PEO–Ba–Si_3N_4 structures. These characteristics include all the electronic, translational, rotational, vibrational and total thermal degrees of freedom.

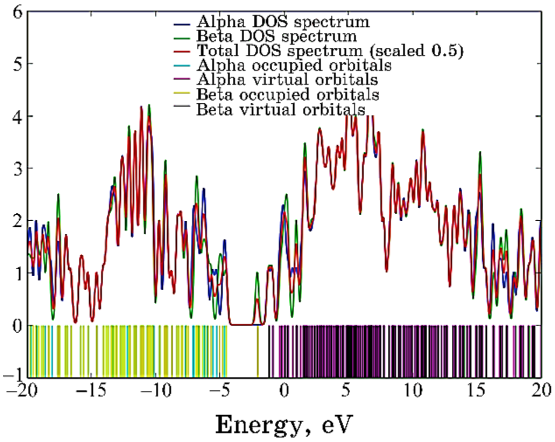

Fig. 8. DOS for PVA–PEO–Ba–Si_3N_4 structure.

TABLE 5. E_{th}, C_v and S_{th} of PVA–PEO–Ba–Si_3N_4 structure.

Thermal corrections, Hartree/partical scheme			
E_{th}, kcal/mol		C_v, cal/(mol·K)	S_{th}, cal/(mol·K)
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	45.147
Rotational	0.889	2.981	38.177
Vibrational	351.958	135.902	176.463
Total	353.736	141.864	261.165

5. CONCLUSIONS

This work included exploring the structure, thermal, optical and electronic characteristics for electronics and optics devices. By using the DFT method, a good relaxation of the PVA–PEO–Ba–Si_3N_4 structures was determined. The ionization potential is greater than the electron affinity; so, the studied structure needs high energy to become cation. According to the high of the electrophilicity, the PVA–PEO–Ba–Si_3N_4 structures are more reactive. The results showed that the PVA–PEO–Ba–Si_3N_4 structures have good optical and electronic properties. In addition, the designed nanostructures have wide absorption spectrum that makes the PVA–PEO–Ba–Si_3N_4 structures as suitable in various electronics devices like transistors, photovoltaic cell, sensors and other devices.

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