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Exploring the Optical Properties of $BaTiO_3$/CuO-Nanoparticles-Doped PVA Polymer for Optoelectronic Applications

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This study aims to prepare of barium titanate ($BaTiO_3$)/copper oxide (CuO)-nanoparticles-doped polyvinyl alcohol (PVA) as new optical material, which can be used in variety optoelectronics applications with a few cost, lightweight, excellent optical properties, and high efficiency. We investigate the impact of the barium titanate and copper oxide nanoparticles with different concentrations 0, 2, 4, and 6 wt.% on polyvinyl alcohol. The solution casting process is used to fabricate the samples. The optical properties findings show that the optical conductivity, complex dielectric constant (with real and imaginary parts), extinction coefficient, absorption, absorption coefficient, and refractive index increase with increasing of $BaTiO_3$–CuO-nanoparticles' concentration, while the optical energy gap and transmittance decrease. This behaviour makes it suitable for several optical nanodevices. In the end, it is clear that the PVA–$BaTiO_3$–CuO nanostructures have useful optical characteristics for applications related to optics and electronics.

Це дослідження спрямоване на одержання леґованого наночастинками титанату Барію ($BaTiO_3$)/оксиду Купруму (CuO) полівінілового спирту (ПВС), оскільки новий оптичний матеріял може бути використаний у різноманітних оптоелектронних застосуваннях із невеликою ціною, малою вагою, чудовими оптичними властивостями та високою ефективністю. Досліджено вплив наночастинок титанату Барію й оксиду Купруму різної концентрації у 0, 2, 4 та 6 мас.% на полівініловий спирт. Для виготовлення зразків використовувався процес лиття розчину. Результати стосовно оптичних властивостей показали, що оптична провідність, діелектрична проникність (як реальна, так і уявна), коефіцієнт екстинкції, поглинання, коефіцієнт поглинання та показник заломлення — все це підвищується зі збільшенням концентрації наночастинок

$BaTiO_3$–CuO, тоді як оптична енергетична щілина та пропускна здатність зменшуються. Така поведінка робить це придатним для ряду оптичних нанопристроїв. Зрештою, було зрозуміло, що наноструктури ПВС–$BaTiO_3$–CuO мають корисні оптичні характеристики для застосування в оптиці й електроніці.

Key words: PVA, barium titanate, copper oxide, nanocomposites, optical properties.

Ключові слова: полівініловий спирт, титанат Барію, оксид Купруму, нанокомпозити, оптичні властивості.

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1. INTRODUCTION

Recent years have seen a surge in interest in nanocomposites. Significant attempts are being made to regulate anon the structures using cutting-edge synthetic methods [1]. Nanocomposites' properties are influenced not only by those methods, not just by the morphology and interfacial properties of their component parents, but also by the composite itself. Unlike the qualities of matter at the level of individual particles or molecules, anon. materials have unique physical, chemical, and biological characteristics. Nanotechnology has made it feasible to modify the melting point, magnetic characteristics, charge capacity, and even colour of materials without altering their chemical makeup [2, 3].

Nanotechnology typically involves the creation of materials or devices with dimensions between 1 nm and 100 nm in at least one dimension. It is possible to approach nanotechnology from either the top down, in which case large structures are broken down into smaller ones (as in the case of photonic applications in nanoelectronics and nan engineering) or the bottom up, in which case atoms and molecules are transformed into nanostructures that are more akin to biological systems [4, 5]. Research in nanotechnology is massive because of how important it will be to society in the 21st century. It is possible that brand-new software will soon be accessible [6, 7].

Many potential nanotechnology's uses stem from the fact that macroscopic and submicroscopic applications of nanoscale structural characteristics exhibit strikingly diverse physical, chemical, and biological properties [8].

The polyvinyl alcohol (PVA) is one of the first and most extensively distributed polymers, and it finds extensive usage in semiconductor applications today. PVA dissolves quickly in water and in organic compounds, which contain hydroxyl groups [9, 10]. PVA is often considered a superior host medium for a variety of nanoparticles. The need to create films with superior transparency and optical properties is the driving force. Their dielectric characteristics, particularly, their flexibility and robustness, have garnered a lot of interest. The flexible ceramic powder barium titanate ($BaTiO_3$) is a ferroelectric that has attracted a lot of interest as a transducer in polymer nanocomposite films due to its high dielectric properties [11, 12]. Copper oxide has an important place among the metal oxides. Despite being the most basic copper molecule, CuO has many desirable features, including high-temperature superconductivity, electronic correlation, and non-toxicity. Crystal structure with a tiny band gap gives it promising photovoltaic and photoconductive capabilities [13, 14]. This paper deals with the preparation and optical characteristics of PVA–$BaTiO_3$–CuO nanostructures for use in different optoelectronic fields.

2. EXPERIMENTAL WORK

PVA–$BaTiO_3$–CuO nanocomposites were made of PVA, barium titanate ($BaTiO_3$) and copper oxide (CuO) by using the solution casting method. Polyvinyl alcohol (PVA) was dissolvent in 40 ml of distilled water, to get a more homogenous solution by swirling with a magnetic stirrer at 75°C for 45 minutes. Barium titanate ($BaTiO_3$) and copper oxide (CuO) nanoparticles have been added to the PVA at concentrations of 2, 4, and 6 wt.%. The optical features of PVA–CuO–$BaTiO_3$ nanostructures were investigated by using a Shimadzu-UV-1800-spectrophotometer in the wavelength range 200–800 nm.

The absorbance A is calculated from equation by [15] as follows:

$$A = \frac{I_a}{I_0},$$

where I_0 is the intensity of incident light, I_a denotes the intensity of light that is absorbed by the medium.

Transmittance T is calculated using the equation by [16]:

$$T = 10^{-A}.$$

The absorbance coefficients α is calculated using the equation by [17]:

$$\alpha = \frac{2.303A}{t},$$

where t is thickness of sample.

Optical energy gap is determined by [18] as follows:

$$B\left(h\nu - E_g^{opt.}\right)^r = \alpha h\nu ,$$

where B is constant; $h\nu$ indicates the photon energy, and $E_g^{opt.}$ is the optical energy gap when $r = 3$ (for the forbidden indirect transition) and $r = 2$ (for the allowed indirect transition).

The extinction coefficient k is obtained by [19] with equation:

$$k = \frac{\alpha\lambda}{4\pi} ,$$

where the wavelength is λ.

Refractive index n is given by [20] as follows:

$$n = \sqrt{4R - \frac{k^2}{(R-1)^2}} - \frac{(R+1)}{(R-1)} ,$$

where R is reflection.

The dielectric constant has real and imaginary parts (ε_1, ε_2). Each of these parts may be determined by [21, 22] using the formulae:

$$\varepsilon_1 = n^2 - k^2 , \ \varepsilon_2 = 2nk .$$

The optical conductivity σ is calculated by [23] using the equation:

$$\sigma = \frac{\alpha n c}{4\pi} .$$

3. RESULTS AND DISCUSSION

Figure 1 shows how PVA–$BaTiO_3$–CuO nanocomposites absorb light at various wavelengths. As can be seen in this figure, the absorbance is decreased with increasing wavelength and is increased with increasing of concentration of nanoparticles. This behaviour can be attributed to the interaction of composite materials with atoms, which ultimately leads to the transmission of photons. At shorter wavelengths, particularly, in proximity to the fundamental absorption edge, a phenomenon arises, wherein the incident photon and material interact, leading to the absorption of the photon. The positive correlation between the weight percentages of $BaTiO_3$–CuO nanoparticles and the absorbance values can be attributed to the absorption of incident light by free electrons [24, 25].

Figure 2 shows how PVA–$BaTiO_3$–CuO nanocomposites' transmittance varies with wavelength. This graph shows that the transmittance decreases with increasing of $BaTiO_3$–CuO-nanoparticles' concentration. This is because the $BaTiO_3$–CuO nanoparticles add elec-

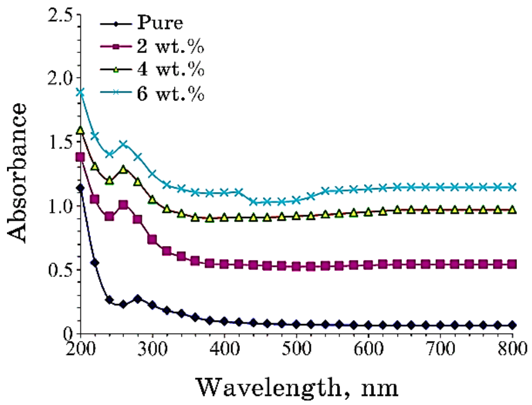

Fig. 1. Connection between absorption and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

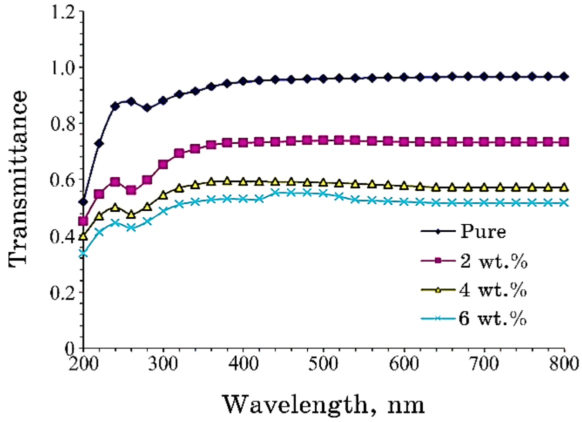

Fig. 2. Connection between transmittance and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

tron, which has occupied unoccupied energy band positions after being transported to a higher energy level; so, the process does not lead to outer-orbital electron emission, where the electrons are vulnerable to electromagnetic forces radiation [26]. Pure PVA, on the other hand, has a low permeability and a high transmittance, allowing docents to pass through it, while absorbing part of the incident light. This is because an electron bond must be broken in order for it to transition to the conduction band, requiring a high-energy photon [27].

Figure 3 shows variation of absorbance coefficient with photon energy for PVA–$BaTiO_3$–CuO nanocomposites. We can observe that, since the incoming photon lacks the necessary energy to move the electron from the valence band (V.B) to the conduction band (C.B), hence, the absorption coefficient is the smallest at high wavelength and low energy. Larger absorption at higher energies is indicative of an abundance of possible electron transitions. In order to move the electron from the V.B to the C.B, the incoming photon must have energy greater than this prohibited energy difference [28, 29]. Since a direct transition of an electron is predicted, the nature of an electron transmission is affected by the absorption coefficient, which is substantial (> 10^4 cm^{-1}) at high energies, when the energy and moment are maintained by the (electrons and photons). In a phonon-mediated indirect transition, the electronic momentum of an electron is likely to be retained [30, 31], since absorption coefficients are (of 10^4 cm^{-1}) at low energies.

Absorbance data for PVA–$BaTiO_3$–CuO nanocomposites reveal

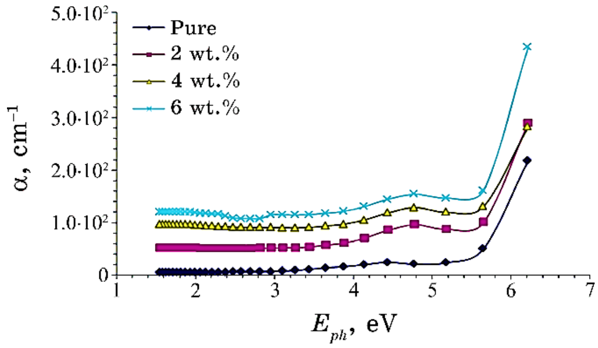

Fig. 3. Connection between absorption coefficient and photon energy for PVA–$BaTiO_3$–CuO nanocomposites.

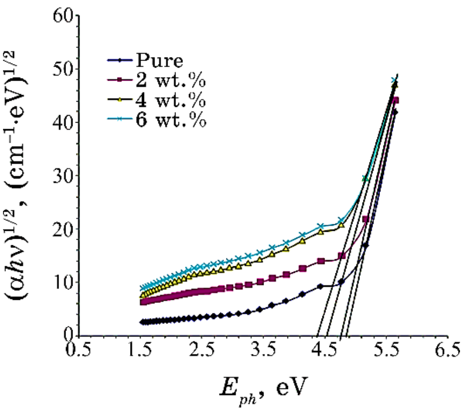

Fig. 4. Connection between absorption edge $(\alpha h\nu)^{1/2}$ and photon energy for PVA–$BaiTO_3$–CuO nanocomposites.

that the electron transition occurs at wavelengths of less than 10^4 cm^{-1}.

Figure 4 shows the relationship between $(\alpha h\nu)^{1/2}$ and photon energy for PVA–$BaTiO_3$–CuO nanocomposites. Drawing a straight line from the curve highest point to the axis (x) at the position, when $(\alpha h\nu)^{1/2} = 0$ (allowable), we get an indirect energy-gap transition. From this figure, the optical energy gap decreases by increasing of $BaTiO_3$–CuO-nanoparticles' concentration. This is can be attributed to the density of localized state increased with increasing concentration of $BaTiO_3$–CuO nanoparticles due to the heterogeneous nature of nanocomposites (*i.e.*, electronic conduction depends on the added concentration) [32, 33].

Figure 5 depicts the relation between $(\alpha h\nu)^{1/3}$ and photon energy for PVA–$BaTiO_3$–CuO nanocomposites. A similar approach takes into account the prohibited transition for the indirect energy gap.

Figure 6 shows the relationship between refractive index of PVA–$BaTiO_3$–CuO nanocomposites and wavelength. From this figure, we can see that the refractive index of PVA–$BaTiO_3$–CuO nanocomposites increases with increasing concentration of $BaTiO_3$–CuO nanoparticles. Upon exposure to incident light, a sample exhibiting high refractivity in the UV region will demonstrate a proportional elevation in its refractive-index values [34, 35].

Figure 7 shows the connection between extinction coefficient and wavelength for PVA–$BaTiO_3$–CuO nanocomposites. The extinction coefficient increases with increasing $BaTiO_3$–CuO-nanoparticles' concentration, as seen in this figure. It is because of the higher absorption coefficient. This occurs because the absorption coefficient increases with increasing concentrations of the barium titanate and copper oxide nanoparticles. This result suggests that the structure

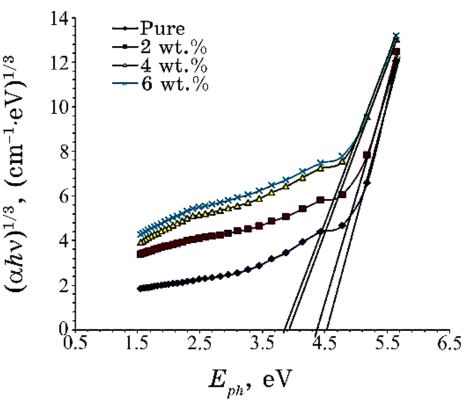

Fig. 5. Connection between $(\alpha h\nu)^{1/3}$ $(cm^{-1}\cdot eV)^{1/3}$ and photon energy for PVA–$BaTiO_3$–CuO.

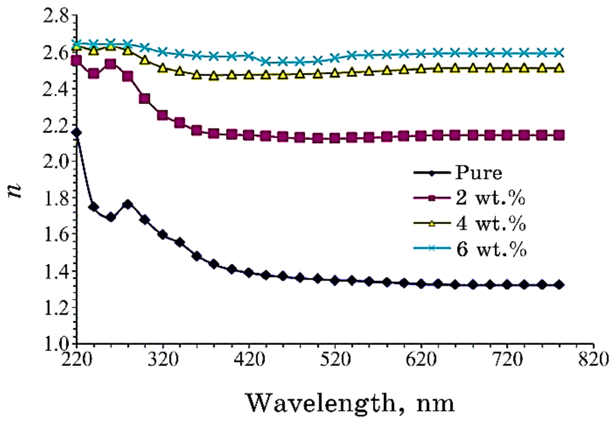

Fig. 6. Connection between refractive index with wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

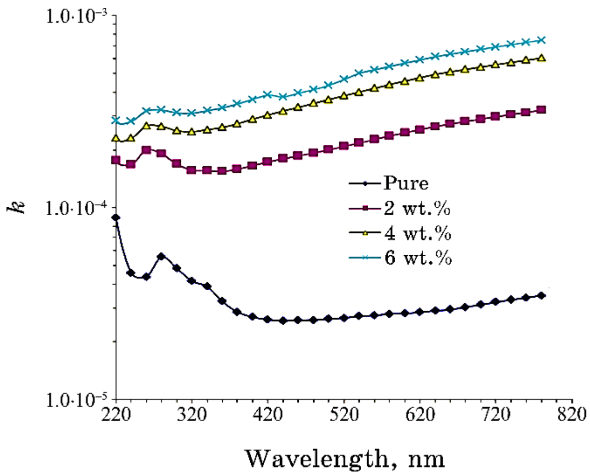

Fig. 7. Connection between extinction coefficient and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

of the polymer will be affected by the presence of $BaTiO_3$–CuO nanoparticles [36, 37].

Figure 8 presents variation of the real part of dielectric constant with wavelength for PVA/$BaTiO_3$/CuO nanocomposites. This figure manifests the real dielectric constant increased with increasing concentrations of $BaTiO_3$–CuO nanoparticles. Because of the smaller value of n^2, this figure demonstrates that ε_1 is highly dependent on k^2 [38, 39].

The relation between wavelength and imaginary part of dielectric constant for PVA/$BaTiO_3$/CuO nanocomposites is displayed in Fig.

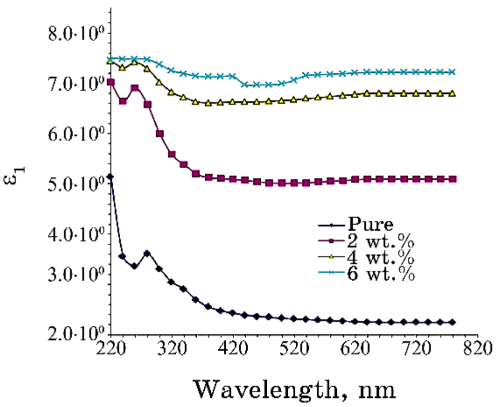

Fig. 8. Connection between real part of the dielectric constant and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

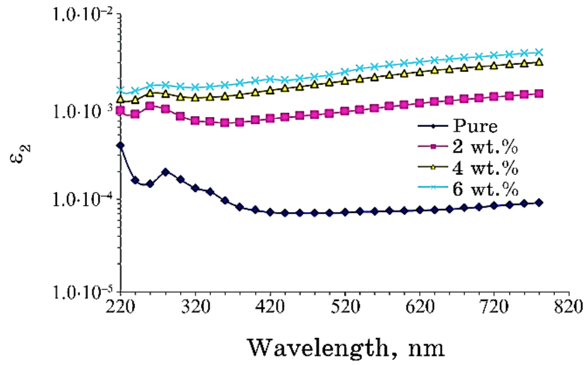

Fig. 9. Connection between imaginary part of dielectric constant and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

9. We can see the imaginary part values, which vary due to the absorption coefficient dependent on k because of their relationship between ε_2 and k. On the other hand, imaginary part of dielectric constant increases with increasing concentration of nanoparticles. Because of the heightened electric polarization induced by the nanoparticles, the rise in electric polarization results in a higher density of dipoles, which, in turn, leads to an increase in the dielectric constant [40, 41].

Figure 10 shows the dependence of optical conductivity of PVA–$BaTiO_3$–CuO nanocomposites on wavelength. Increasing the $BaTiO_3$–CuO proportion in the PVA was shown to increase the optical conductivity. Because the introduction of additional band gap levels facilitates electron transport from the valence band to the conduc-

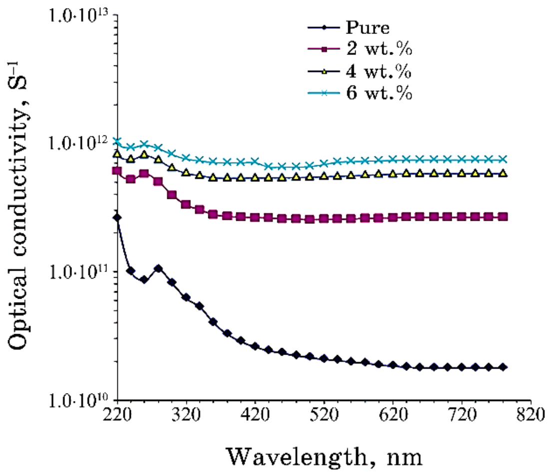

Fig. 10. Connection between optical conductivity and wavelength for PVA–$BaTiO_3$–CuO nanocomposites.

tion band through localized levels, the band gap closes and the conductivity increases as a consequence of this one [42, 43].

4. CONCLUSION

In this paper, the solution casting technique was used to fabricate PVA–$BaTiO_3$–CuO-nanocomposites' films. The optical properties of PVA–$BaTiO_3$–CuO nanostructures have been studied. The optical characteristics showed that the absorption, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric-constant parts, and optical conductivity increase with increasing concentration of $BaTiO_3$–CuO nanoparticles. On the other hand, transmittance and optical energy gap decrease as the concentration of $BaTiO_3$–CuO nanoparticles increases. According to how light interacts with them, nanostructures made of PVA–$BaTiO_3$–CuO are attractive candidates for use in optical and photonic nanodevices.

REFERENCES

1. J. Su and J. Zhang, *Journal of Materials Science: Materials in Electronics*, **30**, No. 3: 1957 (2019); https://doi.org/10.1007/s10854-018-0494-y
2. M. A. Habeeb and Z. S. Jaber, *East European Journal of Physics*, **4**: 176 (2022); doi:10.26565/2312-4334-2022-4-18
3. M. Vinyas and S. C. Kattimani, *Mater. Today Proc.*, **5**: 7410 (2018); https://doi.org/10.1016/j. matpr.2017.11.412
4. A. H. Hadi and M. A. Habeeb, *Journal of Mechanical Engineering Research*

and Developments, **44**, No. 3: 265 (2021); https://jmerd.net/03-2021-265-274
5. Q. M. Jebur, A. Hashim, and M. A. Habeeb, *Egyptian Journal of Chemistry*, **63**: 719 (2020); https://dx.doi.org/10.21608/ejchem.2019.14847.1900
6. M. A. Habeeb, *European Journal of Scientific Research*, **57**, No. 3: 478 (2011).
7. S. Shankar, O. P. Thakur, and M. Jayasimhadri, *Mater. Chem. Phys.*, **234**: 110 (2019); https://doi.org/10.1016/j.matchemphys.2019.05.095
8. S. M. Mahdi and M. A. Habeeb, *Optical and Quantum Electronics*, **54**, Iss. 12: 854 (2022); https://doi.org/10.1007/s11082-022-04267-6
9. N. Hayder, M. A. Habeeb, and A. Hashim, *Egyptian Journal of Chemistry*, **63**: 577 (2020); doi:10.21608/ejchem.2019.14646.1887
10. N. Kumar, V. Crasta, and B. Praveen, *Physics Research International*, **2014**: Article ID 742378-1–9 (2014); https://doi.org/10.1155/2014/742378
11. M. A. Habeeb, A. Hashim, and N. Hayder, *Egyptian Journal of Chemistry*, **63**: 709 (2020); https://dx.doi.org/10.21608/ejchem.2019.13333.1832
12. A. Hashim, M. A. Habeeb, and Q. M. Jebur, *Egyptian Journal of Chemistry*, **63**: 735 (2020); https://dx.doi.org/10.21608/ejchem.2019.14849.1901
13. S. M. Mahdi and M. A. Habeeb, *Physics and Chemistry of Solid State*, **23**, No. 4: 785 (2022); doi:10.15330/pcss.23.4.785-792
14. S. Muntaz Begum, M. Rao, and R. Ravikumar, *Journal of Inorganic and Organometallic Polymers and Materials*, **23**: 350 (2013); https://doi.org/10.1007/s10904-012-9783-8
15. M. A. Habeeb and W. S. Mahdi, *International Journal of Emerging Trends in Engineering Research*, **7**, No. 9 : 247 (2019); doi:10.30534/ijeter/2019/06792019
16. M. A. Habeeb and R. S. Abdul Hamza, *Journal of Bionanoscience*, **12**, No. 3: 328 (2018); https://doi.org/10.1166/jbns.2018.1535
17. Q. Zhang, K. Zhang, D. Xu, G. Yang, H. Huang, F. Nie, C. Liu, and S. Yang, *Progress in Materials Science*, **60**: 208 (2014); https://doi.org/10.1016/j.pmatsci.2013.09.003
18. M. A. Habeeb, A. Hashim, and N. Hayder, *Egyptian Journal of Chemistry*, **63**: 697 (2020); https://dx.doi.org/10.21608/ejchem.2019.12439.1774
19. M. A. Habeeb and W. K. Kadhim, *Journal of Engineering and Applied Sciences*, **9**, No. 4: 109 (2014); doi:10.36478/jeasci.2014.109.113
20. M. Hdidar, S. Chouikhi, A. Fattoum, M. Arous, and A. Kallel, *Journal of Alloys and Compounds*, **750**: 375 (2018); https://doi.org/10.1016/j.jallcom.2018.03.272
21. M. A. Habeeb, *Journal of Engineering and Applied Sciences*, **9**, No. 4: 102 (2014); doi:10.36478/jeasci.2014.102.108
22. H. J. Park, A. Badakhsh, I. T. Im, M.-S. Kim, and C. W. Park, *Applied Thermal Engineering*, **107**: 907 (2016); https://doi.org/10.1016/j.applthermaleng.2016.07.053
23. S. M. Mahdi and M. A. Habeeb, *Digest Journal of Nanomaterials and Biostructures*, **17**, No. 3: 941 (2022); https://doi.org/10.15251/DJNB.2022.173.941
24. G. A. Eid, A. Kany, M. El-Toony, I. Bashter, and F. Gaber, *Arab. J. Nucl. Sci. Appl.*, **46**, No. 2: 226 (2013).
25. A. H. Hadi and M. A. Habeeb, *Journal of Physics: Conference Series*, **1973**:

No. 1: 012063 (2021); doi:10.1088/1742-6596/1973/1/012063
26. Q. M. Jebur, A. Hashim, and M. A. Habeeb, *Egyptian Journal of Chemistry*, **63**, No. 2: 611 (2020); https://dx.doi.org/10.21608/ejchem.2019.10197.1669
27. R. Grigalaitis, M. M. Vijatović Petrović, J. D. Bobić, A. Dzunuzovic, R. Sobiestianskas, A. Brilingas, and B. D. Stojanović, *J. Banys Int.*, **40**: 6165 (2014); https://doi.org/10.1016/j.ceramint.2013.11.069
28. M. A. Habeeb and A. H. Mohammed, *Optical and Quantum Electronics*, **55**, Iss. 9: 791 (2023); https://doi.org/10.1007/s11082-023-05061-8
29. M. H. Dwech, M. A. Habeeb, and A. H. Mohammed, *Ukr. J. Phys.*, **67**, No. 10: 757 (2022); https://doi.org/10.15407/ujpe67.10.757
30. R. N. Bhagat and V. S. Sangawar, *Int. J. Sci. Res. (IJSR)*, **6**: 361 (2017).
31. Z. S. Jaber, M. A. Habeeb, and W. H. Radi, *East European Journal of Physics*, **2**: 228 (2023); doi:10.26565/2312-4334-2023-2-25
32. R. Dalven and R. Gill, *J. Appl. Phys.*, **38**, No. 2: 753 (1967); doi:10.1063/1.1709406
33. V. Suryawanshi, A. S. Varpe, and M. D. Deshpande, *Thin Solid Films*, **645**: 87 (2018); https://doi.org/10.1016/j.tsf.2017.10.016
34. R. S. Abdul Hamza and M. A. Habeeb, *Optical and Quantum Electronics*, **55**, Iss. 8: 705 (2023); https://doi.org/10.1007/s11082-023-04995-3
35. A. Goswami, A. K. Bajpai, and B. K. Sinha, *Polym. Bull.*, **75**, No. 2: 781 (2018); https://doi.org/10.1007/s00289-017-2067-2
36. A. A. Mohammed and M. A. Habeeb, *East European Journal of Physics*, **2**: 157 (2023); doi:10.26565/2312-4334-2023-2-15
37. I. Oreibi and J. M. Al-Issawe, *Turkish Computational and Theoretical Chemistry*, **7**, No. 2: 12 (2023); https://doi.org/10.33435/tcandtc.1161253
38. M. A. Habeeb and R. S. A. Hamza, *Indonesian Journal of Electrical Engineering and Informatics*, **6**, No. 4: 428 (2018); doi:10.11591/ijeei.v6i1.511
39. N. K. Al-Sharifi and M. A. Habeeb, *East European Journal of Physics*, **2**: 341 (2023); doi:10.26565/2312-4334-2023-2-40
40. S. Lather, A. Gupta, J. Dalal, V. Verma, R. Tripathi, and A. Ohlan, *Ceram. Int.*, **43**: 3246 (2017); https://doi.org/10.1016/j.ceramint.2016.11.152
41. M. A. Habeeb and W. H. Rahdi, *Optical and Quantum Electronics*, **55**, Iss. 4: 334 (2023); https://doi.org/10.1007/s11082-023-04639-6
42. S. M. Mahdi and M. A. Habeeb, *AIMS Materials Science*, **10**, No. 2: 288 (2023); doi:10.3934/matersci.2023015
43. C. V. Reddy, B. Babu, I. N. Reddy, and J. Shim, *Ceramics International*, **44**, No. 6: 6940 (2018); https://doi.org/10.1016/j.ceramint.2018.01.123