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Effect of dopant of aluminum on the structural and optical properties of NiTsPc thin films

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The (NiTsPc) thin films operating by vacuum evaporation technique are high recital and good desirable for number of applications, were dumped on glass substrates at room temperature with (200±20nm) thickness and doped with Al at different percentage (0.01,0.03) besides annealing the sample with 200˚C for 1 hours . The stimuluses of aluminum dopant percentage on characterization of the dropped (Ni Ts Pc) thin films were studied through X-ray diffraction in addition from the attained results, were all the films have polycrystalline in nature, as well the fallouts of XRD aimed at film illustrations polycrystalline, depending on the Al ratio doping, the results, SEM exposed the surface is regularly homogeneous. Utilizing first-ideologies calculations, we demonstration that appropriate band gaps and optical properties adjacent to that of direct energy gap intended for wholly samples.

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Keywords: NiTsPc, Thin film, Vacuum evaporation, Doping

1. Introduction

Phthalocyanines (Pcs) organic semiconductor utilized by means of an optoelectronic device [1], molecular materials have explored in place of energetic layers in the manufacture of electronics devices. (Pcs) is an organic, bulky, aromatic compound without the theoretic or dedicated curiosity. Moreover, itis calm fourisoindole pieces related through nitrogen atoms. H_2Pc obligates two-dimension geometrical plus a sphere organization entailing of 18 π-electrons, the conjugate dishonorable of H2Pc, stand appreciated in organic solar cells, and photodynamic therapy. Substantial exploration on H_2Pc and MPc resultant in a varied series of applications in areas excluding catalysis, photo dynamic therapy and nano particle structure [2]. The electronic chemical possessions of MPc brand active electron donor too acceptor. Accordingly, organic solar cells thru influence adaptation efficiencies on otherwise underneath (5%) need industrialized [3,4]. Likewise, MPcs used by way of catalysts designed for the oxidation of methane, phenols, alcohols, polysaccharides, and olefins, also utilized to catalyze C–C bond creation then countless discount reaction [5]. Zinc phthalo cyanine besides silicon industrialized in place of photo sensitizers [6]. Several (MPcs) exposed the capability to arrangement nano structure which require potential applications in electronical and bio sensing [7-9]. Testimony (Pcs) films are habitually approved via the conservative thermal evaporation technique, where identified as an involved method since greatest of pure MPcs were not solvable in slightly organic solvent [10,11]. The intention of contribution the MPcs to liquefy in solvent in addition to augment themobility of the charge carrier in electronic devices, dissimilar function clusters have been announced to the Pcs. [12], for sensor applications the NiPc derivative, nickel (II) phthalo cyaninete

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trasulfonic acid tetrasodium salt (NiTSPc) was investigated, which indicated the augmentation of the electrically property of (NiPc) through ascribing a tetra sulfonic function set[13]. In the paper case, we present our results on the deposit NiTsPc thin films thru thermal evaporation practice. The stimulus of Al doping on NiTsPc films, structural optical, and morphological properties were studied.

2. Experiment Procedures

NiTsPc films with thickness (200nm) were deposited via vacuum evaporation method scheduled glass substrate and on (111) p- type Si wafers. Earlier deposited glass substrate be there cleaning. The source to substrate detachment throughout vacuum statement of the film be located (15 cm), utilizing quartz crystal thickness monitor for measured film thickness. The evaporation progression was approved in approximately indistinguishable deposition situations. Fallouts of the X-ray diffraction are inveterate for thin films using Cu Kα radiation (k = 1.542A ˚). The optical absorption property be situated explored per spectrophotometer model UV-1800 series. Also, by way of using a scanning electron microscope (JEOL, JSM 840) unit, superficial morphology of the deposits be present investigated. Aluminum was doped to enhance the electrical properties of the NiTsPc films by thermal diffusion method with ratio (0.01, 0.03). A rotational motivation was active to preserve regularity in film thickness then come to be well distribution of Al into NiTsPc films, models be located at annealing in a hot air range at (200˚C) designed for 1 hours.

3. Results and discussion

From diffraction peaks the regular crystal size container by premeditated utilizing Scherrer comparison [14]. Beginning from figure (1) the consequence of Al dopant and annealing temperature scheduled the structural property of deposited (Ni Ts Pc) thin films was exposed. It is perceptibly detected that entirely thin films equipped ought to polycrystalline, similarly the intensity of wholly diffraction peaks intensification with intensification the Al proportion , by reason of the augmentation of the crystal structural plus the crystallinity convert well .

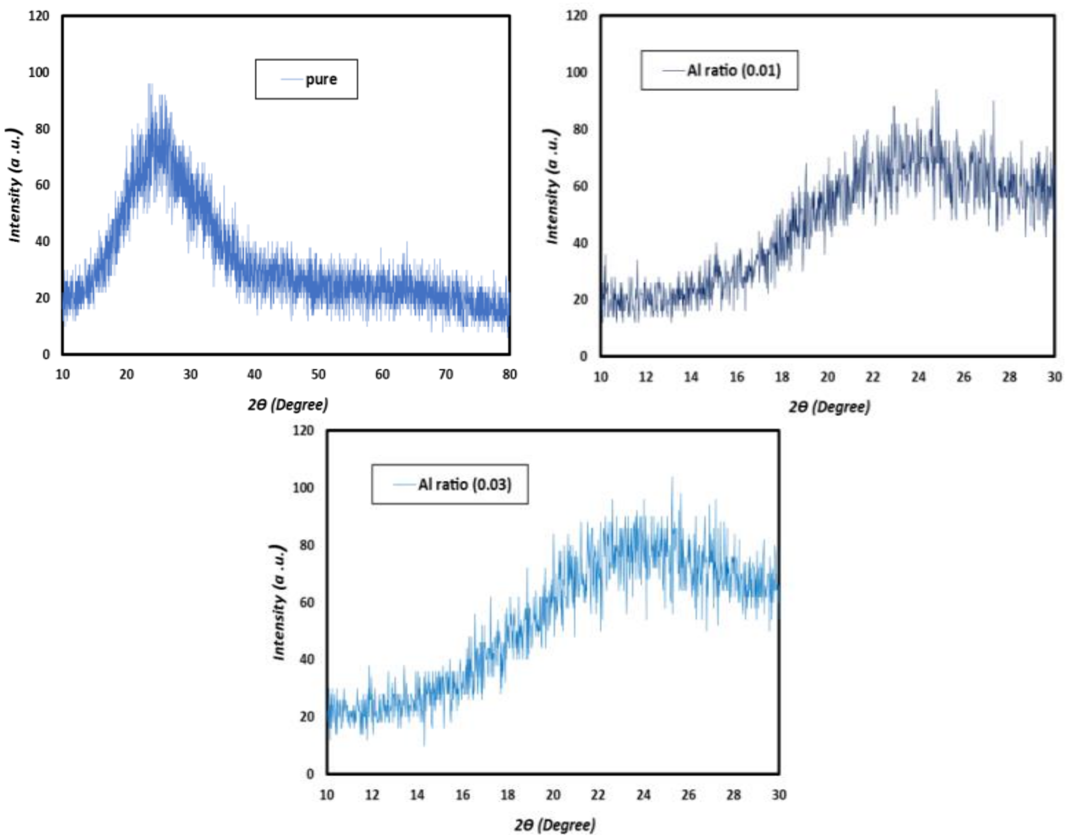

Fig. 1. XRD patterns gotten for the NiTsPc thin films doping with different Al ratio, annealing with (473 K).

Moreover, annealing temperature (473K) given that energy to crystallites in advance sufficient energy to orient in exact stability sites, consequential decrease in grain boundaries, dislocation density ,and the number of crystals are calculated by using the equations [15, 16] . From table (1), we found that Al ratio and annealing have extraordinary impact on the crystallinity, demonstrating that doping (Al with 0.03 ratio) make crystalline size increase although the dislocation density plus quantity of crystals diminution through upsurge dopant percentage as shown in figure (2).

Table 1. Characterizes the consequences of X-ray of NiTsPc thin films doping with different Al ratio, annealing with (473 K).

doping Al concentration	d (A°)	**2θ**	FWHM	G.S 9nm)
0	3.683123	24.1427	1.o6000	80.075
0.01	3.77699	25.803	0. 92000	92. 48
0.03	3.504902	23.5340	0.72000	117.75

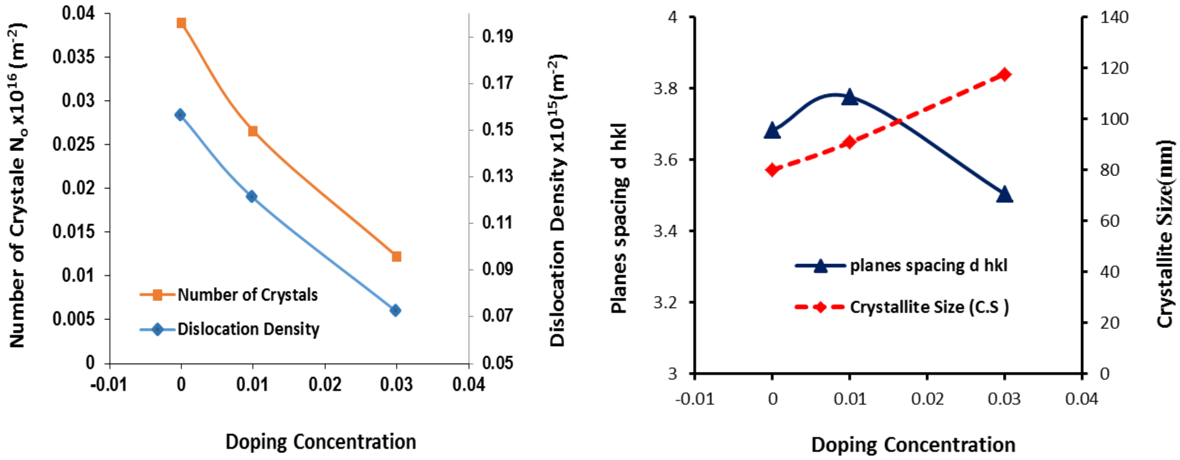

Fig. 2. XRD patterns characterizes the results of X-ray for NiTsPc thin films, annealing with (473) K.

Fig. 3 shows imageries of superficial micro graphic as a result of used scan electron microscopy (SEM) of the pure and Al- doping NiTsPc thin films, analysis of crystal morphology illustrates this, structure closely packed to each other indicating that all films have homogenous distribution and fine grained morphology with intensification in nucleation over growth , by influence of the annealing , furthermore perceived unvarying grain size besides exhibition growing of small grains with increase atomic doping ratio, these results are compatible with XRD consequences.

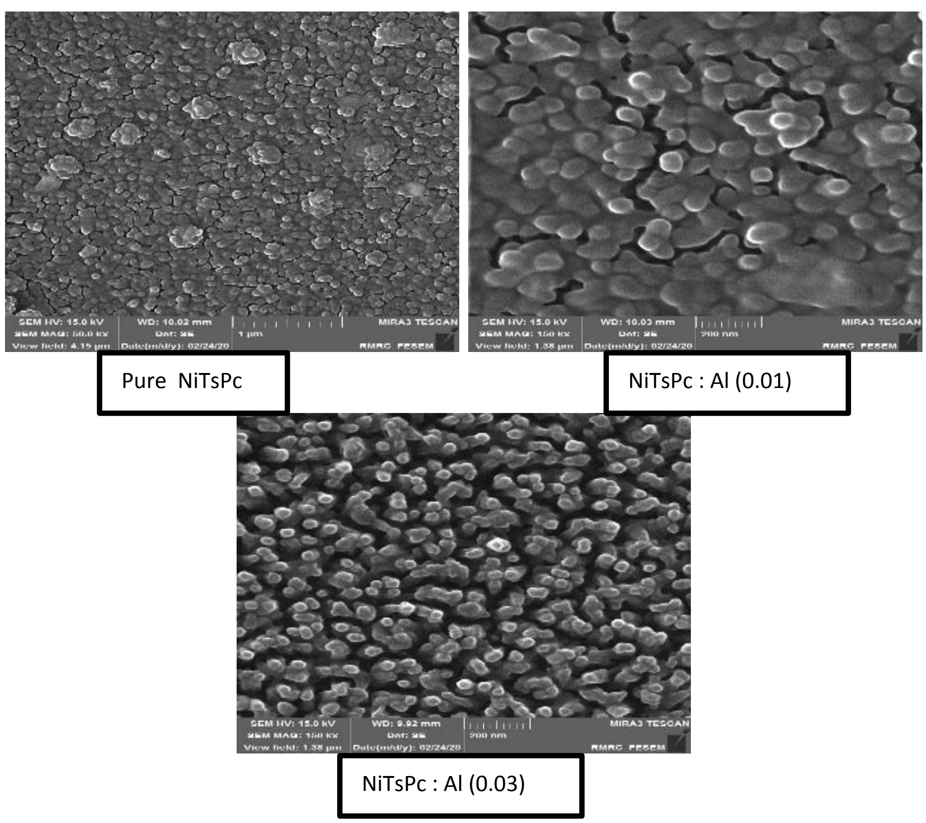

Fig. 3. SEM micrograph for NiTsPc thin films, annealing with (473) K.

The absorption spectrum be governed by the energy quantity of the levels, which in turn are associated to the crystalline and chemical composition of the substance absorption that restrained in place of occupation of wave length (400-1100) nm. Fig (4) represent the change of the absorbance variety of the wavelength, where absorption increases when Al concentration increases, we explained by the increase in crystallite and due the growing of crystallite remained repressed since a acceptable structural which incomes films variations in prearrangement then spreading of atoms in crystal structure subsequently dopant . In addition to, we exhibition that films have an absorption edge which modifications near advanced wavelength afterward doping and that similar to the previous studies [17,18].

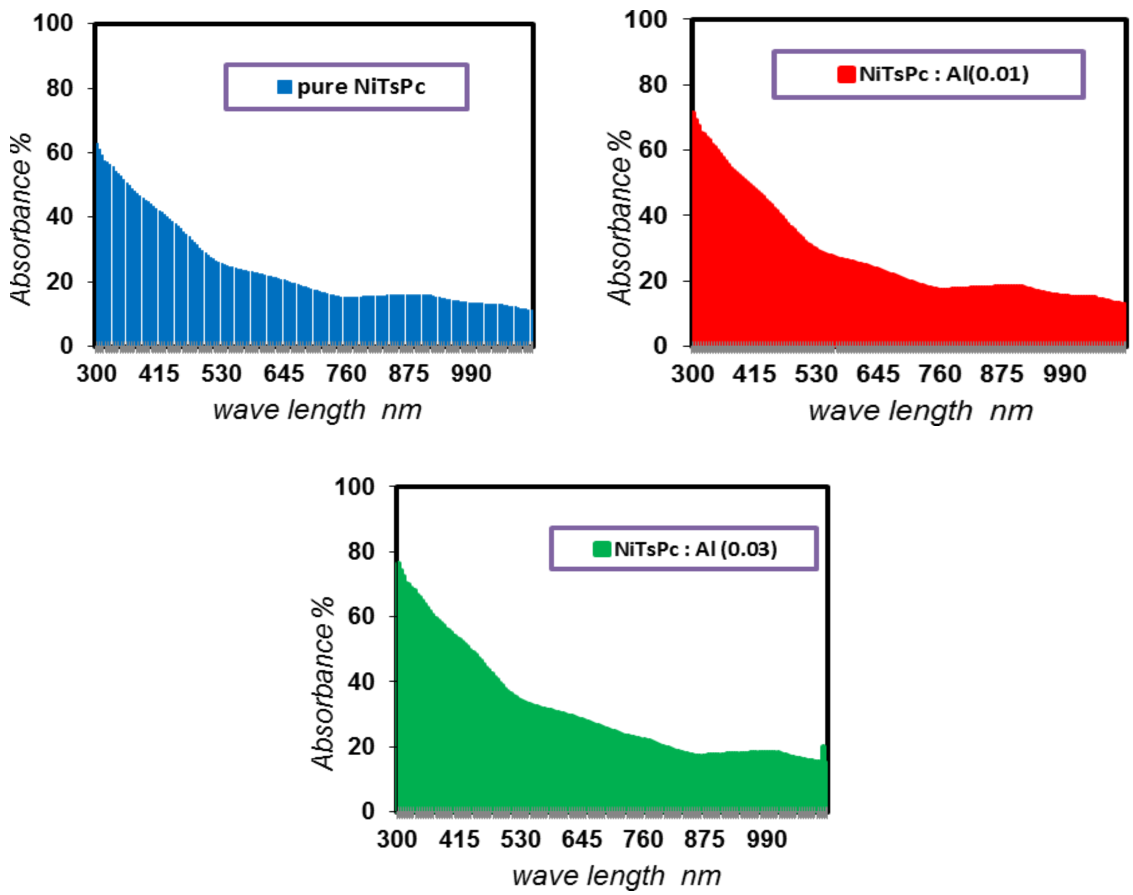

Fig. 4. Absorption spectra for NiTsPc films deposited on diverse Al ratio.

Additional examination of the optical energy gap requires completed via scheming the Tauc plots utilized Tauc's relative [19,20] , the optical property information was based on calculate of band gap energy Eg, fig 5.

The behavior of absorbance related to the changes in crystal structure of these films after annealing, in addition to the optical energy gap reduction per cumulative concentration by reason of that dopant atom introduces inter band energy levels in the band gap of thin films which centrals toward change near subordinate band gap energy, similar results from NiTsPc thin films deposited on glass substrate [21, 22]. Besides, films ought to high values ($\alpha > 10^4$ cm^{-1}), this designated that the direct transition was happen, and the value of optical absorption coefficient (α) rise through intensification Al dopants which is demonstrate in fig 6.

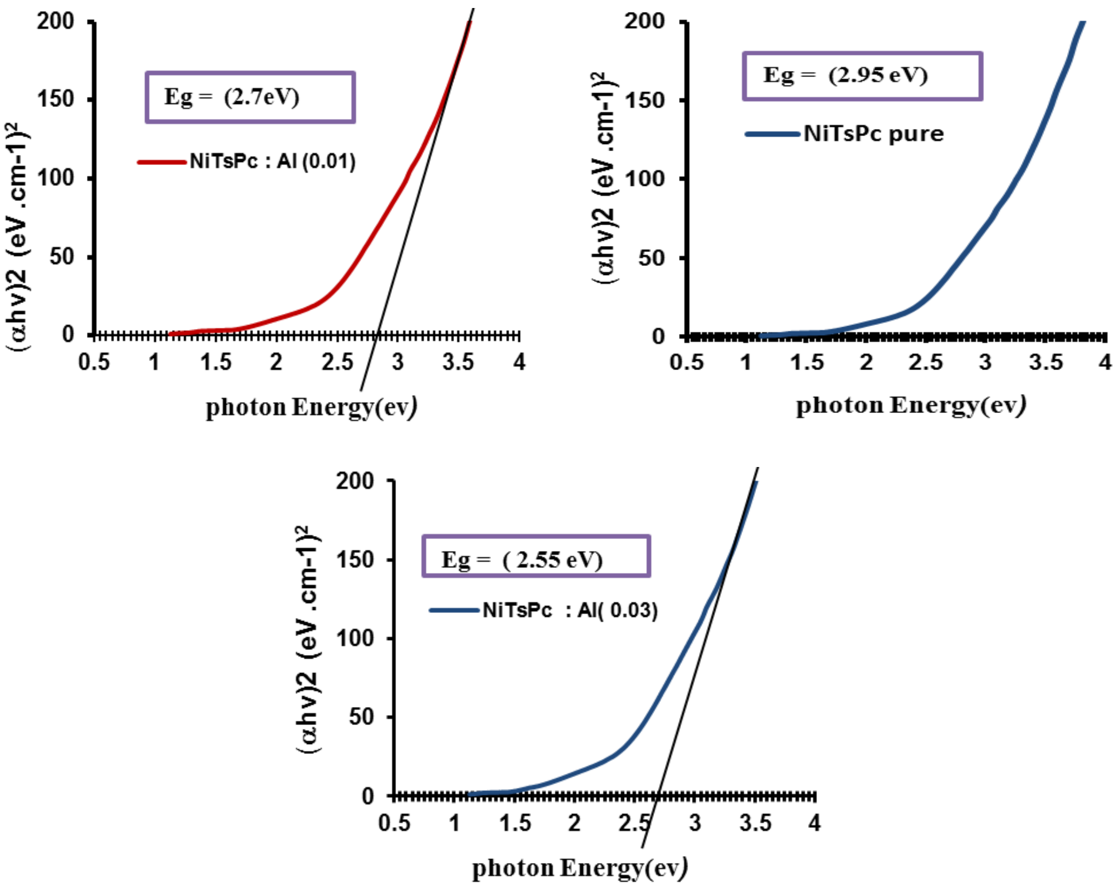

Fig. 5. Disparity of $(ahv)^2$ vs. photon energy for NiTsPc thin films deposited on unalike Al percentage.

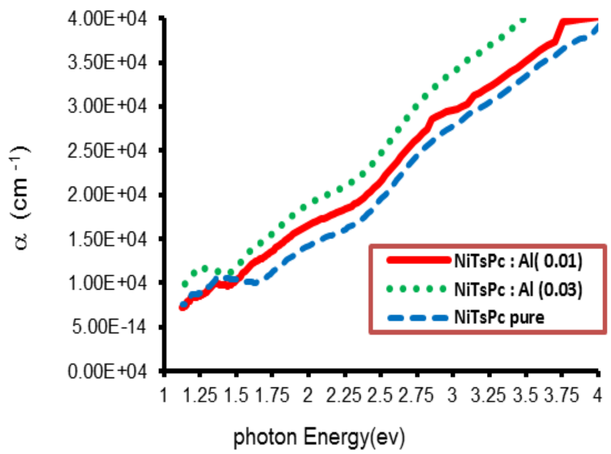

Fig. 6. Deviation of absorption coefficient in competition with Photon energy for for NiTsPc thin films deposited on diverse Al quotient.

4. Conclusion

NiTsPc thin films were depositing through vacuum evaporation system. The structural in addition optical studies of NiTsPc thin films deposited were examined then from the gotten consequences it was detected that the different doping ratio of Al required high influence on the optical and structural properties of the thin films. The NiTsPc thin films deposited with Al (0.03)and (473 K) annealed, had the higher growth rate, better crystallinity , SEM exposed the surface of the film is regularly homogeneous, the optical measurement showed direct allowed per usual band gap energies differs in the variety of (2.55 -2.95) eV with conversion deposition parameter. Probabilities to realize p-type doping canister be developed by scheming evolution situations that undermine the establishment of recompensing centers, where significant in optical device applications.

References

[1] Dahlen Miles A., Industrial & Engineering Chemistry. 31 (7): 839-847, (1939); https://doi.org/10.1021/ie50355a012

[2] Claessens, Christian G.; Hahn, Uwe; Torres, Tomás " The Chemical Record. 8 (2): 75-97, (2008); https://doi.org/10.1002/tcr.20139

[3] Kumar, Challuri Vijay; Sfyri, Georgia; Raptis, Dimitrios; Stathatos, Elias; Lianos, Panagiotis, RSC Advances. 5 (5): 3786-3791, (2014); https://doi.org/10.1039/C4RA14321C

[4] Yuen, Avery P.; Jovanovic, Stephen M.; Hor, Ah-Mee; Klenkler, Richard A.; Devenyi, Gabriel A.; Loutfy, Rafik O.; Preston, John S. Solar Energy. 86 (6): 1683-1688. (2012); https://doi.org/10.1016/j.solener.2012.03.019

[5] Sorokin, Alexander B., Chemical Reviews. 113 (10): 8152-8191, (2013); https://doi.org/10.1021/cr4000072

[6] Miller, J; Baron, E; Scull, H; Hsia, A; Berlin, J; Mccormick, T; Colussi, V; Kenney, M; Cooper, K. Toxicology and Applied Pharmacology. 224 (3): 290-299, (2007); https://doi.org/10.1016/j.taap.2007.01.025

[7] Karan, Santanu; Basak, Dhrubajyoti; Mallik, Biswanath, Chemical Physics Letters, 434 (4-6): 265-270, (2007); https://doi.org/10.1016/j.cplett.2006.12.007

[8] Van Keuren, Edward; Bone, Alysia; Ma, Changbao, Langmuir. 24 (12): 6079-6084, (2008); https://doi.org/10.1021/la800290s

[9] Lokesh, K.S.; Shivaraj, Y.; Dayananda, B.P.; Chandra, Sudeshna, Bioelectrochemistry. 75 (2): 104-109, (2009); https://doi.org/10.1016/j.bioelechem.2009.02.005

[10] Joseph B and Menon C S J. Chem. 4 255, (2007); https://doi.org/10.1155/2007/643834

[11] Sharma G D, Balaraju P, Sharma S K and Roy M S, Synthetic Metals,158 (15) 620 (2008); https://doi.org/10.1016/j.synthmet.2008.04.008

[12] Nešpu˙ ek S, Chaidogiannos G, Glezos N, Wang G, Böhm S, Rakušan J and Karásková M, Mol. Cryst. Liq. Cryst. Sci. Technol. 468 3, (2007); https://doi.org/10.1080/15421400701229396

[13] Ahmad Z, Abdullah S M and Sulaiman K Sens. Actuat.A 179 144, (2012); https://doi.org/10.1016/j.sna.2012.03.037

[14] Langford, J.I. and A. Wilson, Journal of Applied Crystallography, 11(2): p. 102-113, (1978); https://doi.org/10.1107/S0021889878012844

[15] Hanan K. Hassun, Samir A. Maki, Ibn Al-Haitham J. for Pure & Appl. Sci. 29 (2) (2016).

[16] A. Efros, Physics State ,Sol. (b) , 76 ,475 ,(1976); https://doi.org/10.1002/pssb.2220760205

[17] M. S. Fakir, Z. Ahmad, and K. Sulaiman, Chinese Phys. Lett., 29 (12), 1-5, (2012); https://doi.org/10.1088/0256-307X/29/12/126802

[18] N. K. Abbas, A. F. Abdulameer, and A. H. Kadhum, Iraqi Journal of Physics 15 (33), 40-48, (2017).

[19] Nassr I Najm, Hanan K Hassun, Bushra KH al-Maiyaly, Bushra H Hussein, Auday H Shaban, AIP Conference Proceedings 2123, 020031 (2019).

[20] B. H. Hussein, H. K. Hassun, B. K.H. Al-Maiyaly and S. H. Aleabi, Journal of Ovonic Research, 18 (1) 37- 42 (2022); https://doi.org/10.15251/JOR.2022.181.37

[21] Fakir, M.S., Z. Ahmad, and K. Sulaiman, Chinese Physics Letters, 29(12) 126802 (2012); https://doi.org/10.1088/0256-307X/29/12/126802

[22] Mohammed Yarub Hania, Addnan H. Al-Aarajiyb, Ahmed M.Abdul-Lettifa, Journal University of Kerbala , 16 (1) Scientific (2018).