



Hybrid Polymer/Metal Oxide Nanocomposites for Application of Combating Antimicrobial Resistance Materials

Abstract: Polyaniline-NiO (PANI-NiO) nanocomposites reinforced with NiO nanoparticles in a polyaniline matrix were successfully manufactured using a simple perfunctory mixing procedure. PANI-NiO nanocomposites were used to describe the intermediates and final products of the nanocomposites using spectroscopic techniques and antimicrobial studies. In addition to studying the chemical structure, optical properties, crystalline nature, heat conductivity, surface morphology, and antibacterial agents, this work provides a straightforward and effective way to control PANI-NiO nanocomposites. The synthesized PANI's conductive emeraldine base form was validated by UV-Vis and FTIR data, the creation of PANI-NiO nanocomposites and the electrical interaction between PANI and NiO was confirmed. X-ray diffraction studies have demonstrated that the PANI matrix and NiO nanoparticles can be successfully incorporated to create hybrid nanocomposites. Scanning electron microscope (SEM) micrographs demonstrated that PANI was effectively enlarged by NiO treatment and that the final nanocomposite had completely exfoliated NiO powders. The thermal stability of the complex was investigated using thermogravimetric analysis, which demonstrated that the polymer nanocomposites increased the thermal stability over pure organic polymers. When the antibacterial activities of the molecules were investigated, PANI-NiO was found to be a highly effective antibacterial agent. The intercalation of PANI into the NiO nanoparticles is thought to be the reason for the increase in antibacterial agents in the PANI-NiO nanocomposites. The above systematic investigation reveals that the NiO nanoparticles in the PANI matrix have a phenomenal effect on determining the important and antibacterial properties of the nanocomposites.

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1.Introduction:

Polymer nanocomposites are tight (almost molecular) pairings of one or more inorganic nanoparticles and polymers that combine the unique qualities of the former and the latter's inherent traits. [1]. Several investigations have been conducted to enhance the techniques for adding nanoparticles to polymeric matrices. In these combinations, the polymer is usually taken in melt or solution form, and the components are usually blended or mixed. Sensors, microelectronics, nonlinear optics, battery cathodes, and other fields have successfully employed the resultant nanocomposites [2]. Since the creation of materials and nanocomposites based on nanoclusters the field of materials science has made considerable strides. A unique class of materials known as nanocomposites is created by skillfully combining several nanosized particles or objects in a particular way. The resulting materials have unique physical characteristics and a broad range of possible applications. The ability of parent elements to successfully combine into a single material has resulted in novel attributes of nanocomposites [3]. However, in every instance, the creation of the nanocomposite necessitates trapping or encapsulation as opposed to merely merging or fusing. The previous class of



nanocomposites, referred to as the "inorganic-in-organic" system, is the subject of this introduction.

Organic-inorganic nanocomposites are often defined as natural polymer nanocomposites with inorganic nanoscale building blocks. Materials for organic-inorganic nanocomposite systems have long been the subject of intensive research, when their inorganic portions reach the nanoscale [4]. The benefits of organic polymer include flexibility, dielectricity, ductility, and processability, whereas those of inorganic materials include stiffness and thermal stability. The production of hybrid nanocomposite materials and manipulation of one or more of the properties of the components are made possible by the molecular combination of two drastically different components. PANI can adopt the shape of hollow spheres, nanorods, nanowires, nanofibers, or nanoparticles. PANI-metal oxide-based nanocomposites have been developed using several methods with metal oxides [5]. In situ chemical oxidative polymerization and In situ electropolymerization were the two methods used to prepare the majority of PANI-metal oxide-based nanocomposites. PANI-metal oxide-based nanocomposites turned out to be prepared by several techniques, including interfacial polymerization, solution mixing, self-assembly approach, Pickering emulsion polymerization, mechanical mixing method, and so on [6]. Owing to their numerous promising technological uses, conducting polymers such as polypyrrole, polyaniline, poly-o-toluidine and polythiophene, consisting of conjugated electronic structures, have recently ignited widespread fascination and novel. antibacterial activity properties have been found in specific conducting polymers, such as polyaniline and its derivatives. [7]. PANI's unique combination of optical, electronic, and magnetic properties which can be tailored to obtain metallic or insulating properties based on its oxidation state and degree of protonation and its typical polymer properties exhibity and processability make it a beautiful material; the easy and reversible acid-base doping-dedoping chemistry of PANI, in contrast to conjugated polymers, confers significant technical value and allows for control over physico-chemical properties including electrical conductivity and optical activity [8]. Nanoparticles and certain nanostructured materials, or templates, are the two main

categories of inorganic materials employed for this purpose. Additionally, nanocomposites are divided into two groups based on how the natural and artificial components associate with one another: inorganic particles implanted in the natural framework and organic polymers confined within the inorganic template. [9].

2. Experimental

2.1 Materials

The main reagents used for the synthesis of the materials were aniline ($C_6H_5NH_2$) (molecular weight 93.13 g mol⁻¹, density 1.02 kg) from Merck Ltd. and- nickel oxide nanoparticles, <50nm (98% purity) from Sigma Aldrich. All other chemicals and reagents, sulfuric acid (H_2SO_4) (molecular weight 98.08 g mol⁻¹, density 1.84 kg), Ammonium Peroxodisulfate ($(NH_4)_2S_2O_8$) (molecular weight 228.20 g mol⁻¹), Acetone (C_3H_6O), Ammonium hydroxide (NH_4OH) were purchased from Merck Ltd. In addition, demineralized water from Nice was used in this study.

2.2 Synthesis of polyaniline & Preparation of polyaniline-NiO nanocomposites

Polyaniline was synthesized using a chemical oxidative polymerization method. Before use, the aniline monomer was purified by distillation at low pressure and refrigerated. The dopant, H_2SO_4 , was dissolved in approximately 250 ml of demineralized water and thoroughly mixed in a round-bottom flask. The suspension solution was agitated for ten minutes following the addition of the aniline monomer. A dark black solution was obtained by adding ammonium peroxydisulfate $(NH_4)_2S_2O_8$ dropwise slowly as an oxidant after 30 min. This process ensures a good degree of polymerization. The final mixture was kept in an ice-water bath for vigorous stirring for an additional reaction time of 24 h and allowed to proceed at (0–5 °C) temperature. The spinning speed is maintained at 700 rpm. The precipitate was then rinsed with ethanol, acetone, and ultra-pure water and dried for 24 hours at 80°C. For the making of Polyaniline-nickel oxide (PANI-NiO) nanocomposites by used

mechanical mixing method, they were made with varying weight percentages of NiO-25%, 50%, and 100% in relation to polyaniline. For the formation of PANI-NiO (25%) nanocomposites, the molar ratio of the polymer (PANI) to NiO was 1:0.25. Likewise, nanosamples with varying weight percentages of NiO, such as PANI-NiO (50%) and PANI-NiO (100%), were blended at ratio of 1:0.50 and 1:1, respectively.

3. Results and Discussion

3.1 FTIR analysis

The main chain composition of the nanocomposites at a low temperature is shown in Figure.1, and the FTIR spectra of the pure PANI and PANI-NiO nanocomposites, and the key distinctive peaks are listed in Table.1. The N-H stretching vibration of the PANI-NiO nanocomposites was measured at 3417 cm^{-1} [10]. The second and third stretching vibrations of the nanocomposites were ascribed to the C=C (benzenoid) and quinoid) vibrations, respectively, at 1590 and 1502 cm^{-1} . The PANI-NiO nanocomposite (100%) exhibited a C=C (quinoid) and C=C (benzenoid) vibrations at 1586 and 1497 cm^{-1} , respectively. In the wavenumber area, there were some fluctuating variations in the quinoid and benzenoid vibrations in the nanocomposite samples. As the peak intensity of the benzenoid vibration increased, the peak intensity of the quinoid stretching vibration decreased. [11]. PANI-NiO (50,100%) nanocomposite FTIR spectra (Fig.1b, 1c) display two prominent bands: 1390 cm^{-1} , 1399 cm^{-1} (C-N stretching (Q=N-B)) and 1307 cm^{-1} , 1310 cm^{-1} (C-N stretching of secondary aromatic amine). With an increase in the dopant concentration of NiO nPs, the peak intensities of C-N stretching (Q=N-B) and C-N stretching of secondary aromatic amines increased [12]. The C-H in-plane bending mode vibration of the PANI-NiO (50,100%) nanocomposites is assigned at 1129 , 1120 cm^{-1} ; Fig1.b and 1c [13] illustrate this bending vibration peak

intensity, which is clearly increased. Similarly, the nanocomposites samples out-of-plane bending vibration of the nanocomposite samples is attributed to 836 and 832 cm^{-1} , and its peak strength increased when the NiO concentration increased [14]. The presence of metal-oxide bonds in the nanocomposite may be indicated by the formation of tiny bands next to $\sim 800\text{--}500\text{ cm}^{-1}$. Ultimately, the low wavenumber side of the Ni-O-Ni stretching vibration is was 615 and 614 cm^{-1} for the 50% and 100% nanocomposites, respectively. When NiO nPs were introduced into the polymer chain, the peak intensity and breadth increased, clearly showing that the PANI chain molecules remained remarkably intact. [15].

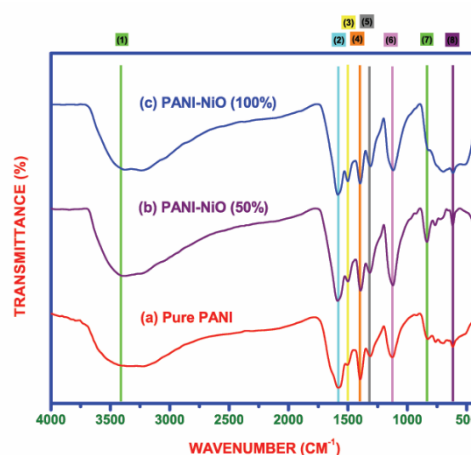


Fig.1 FTIR spectra of pure PANI (a) and PANI-NiO (50, 100%) nCs (b) and (c)

Owing to the metal oxide addition, many of the bands in the PANI sample are actually red-shifted when compared to the nanocomposite [16,17]. The PANI-NiO nanocomposite's spectrum resembled that of pure PANI, but all of the PANI-NiO's prominent peaks moved to lower wavenumbers, indicating that PANI and NiOnPs interact. The characteristic bands of the PANI-NiO nanocomposites In particular, the absence of any new band in the FTIR indicates that the PANI and NiO nanocomposites are not undergoing any chemical reactions. [18].

Table.1 FTIR wavenumber region and parameters of pure PANI and PANI-NiO nCs

Peak No	Vibrations	Parameters	Pure PANI	PANI-NiO (50%)	PANI-NiO (100%)
1	N-H Stretching	Wavenumber (cm ⁻¹)	3417	3417	3417
		Transmittance (%)	53.66	39.65	42.74
2	C=C Stretching Vibration (Quinoid)	Wavenumber (cm ⁻¹)	1586	1590	1586
		Transmittance (%)	34.05	17.07	19.11
3	C=C Stretching Vibration (Benzoid)	Wavenumber (cm ⁻¹)	1499	1502	1497
		Transmittance (%)	54.38	34.17	31.47
4	C-N Stretching (Q=N-B))	Wavenumber (cm ⁻¹)	1399	1390	1399
		Transmittance (%)	41.48	26.22	29.12
5	C-N (secondary aromatic amine)	Wavenumber (cm ⁻¹)	1316	1307	1310
		Transmittance (%)	61.90	42.87	44.88
6	C-H in-plane bending mode	Wavenumber (cm ⁻¹)	1123	1129	1120
		Transmittance (%)	61.00	31.71	40.67
7	C-H out plane bending mode	Wavenumber (cm ⁻¹)	817	836	832
		Transmittance (%)	77.74	69.03	60.28
2	Ni-O-Ni stretching vibration	Wavenumber (cm ⁻¹)	-	615	614
		Transmittance (%)	70.64	83.69	38.24

3.2 UV-Vis Analysis

The UV-visible spectra of PANIs and PANI-NiO nanocomposites exhibited two absorption maxima in the DMSO solution. The UV-visible spectrum of the pure PANI base had two bands at: 328 and 627 nm. The π - π^* electronic transition is due to the band at 328 nm, and its position closely matches that of the typical PANI emeraldine base [19]. The quantity of aniline units affected this band. At a wavelength of 627 nm, the "exciton" band is believed to be the consequence of a charge transfer from the lowest unoccupied energy level, which is centered on the quinonoid ring, to the highest occupied energy level, which is centered on the benzenoid ring. The exciton band, which was measured at 627 nm for the "standard" emeraldine base, ascertained the oxidation state of PANI [20]. The UV-visible spectra of the PANI-NiO (50%) and PANI-NiO (100%) nanocomposites showed two absorption maxima that blue-shifted when the Ni

concentration in the nanocomposites increased from 323 and 622 nm for PANI-NiO (50%) to 321 and 618 nm for PANI-NiO (100%). The blue colour of the solutions of PANI-NiO (50,100%) and pure PANI in DMSO solution indicates that PANI was partially oxidized in the two nanocomposites. The oxidation state of PANI-NiO (50%) is extremely similar to that of pure PANI, that is, the emeraldine base state [21]. This finding suggests that polyaniline and nanocrystalline NiO strongly interact. UV-visible absorption measurements provide a practical and efficient way to examine a few key aspects of semiconductor material band structures. The n-type absorption coefficients of NiO and p-type absorption coefficients of PANI in the PANI-NiO nanocomposites were examined to determine the optical band-gap energies using classical Tauc equation method [22]. It is well known that the following expression, which applies to a wide range of semiconductors, provides the dependence of the absorption coefficient, α , for

the high frequency region on the photon energy, E_p , for optically driven transitions.

$$\alpha E_p = K(E_p - E_g)^n$$

Where K is a constant that varies depending on the type of transition, E_p is the photon energy, and E_g is the optical band gap. For permitted direct, forbidden direct, allowed indirect, and forbidden indirect transitions, the value of the parameter n is $\frac{1}{2}$, $\frac{3}{2}$, 2, and 3, respectively, which takes into consideration the various potential electronic transitions that may be responsible for light absorption [23]. The Tauc plots of $(\alpha E_p)^2$ against E_p for the PANI and PANI-NiO nanocomposites are shown in Fig.3. The optimal match between $(\alpha E_p)^2$ and E_p for both materials was found at $n = 1/2$, indicating permitted direct transitions between the energy band-gaps of PANI-NiO nanocomposites and pure PANI [24]. The optical band-gap energy can be computed using the extrapolated value of E_p at $\alpha=0$, which is the straight line to the x axis; the value for pure PANI (Fig. 3a) is $E_g=3.284$ eV. The values for PANI-NiO (50,100%) nanocomposite (Fig. 3b, 3c) reveal a definite dual band-gap character with $E_g=3.2$ eV and 3.3 eV, respectively [25]. The band gap of pure PANI is nearly the same as that of the PANI-NiO (50,100%) nanocomposite, indicating that intercalated PANI has no discernible impact on PANI's optical band-gap energy of PANI. The absorption peaks of the PANI-NiO nanocomposite blue shifted to shorter wavelengths and resembled those of PANI [26].

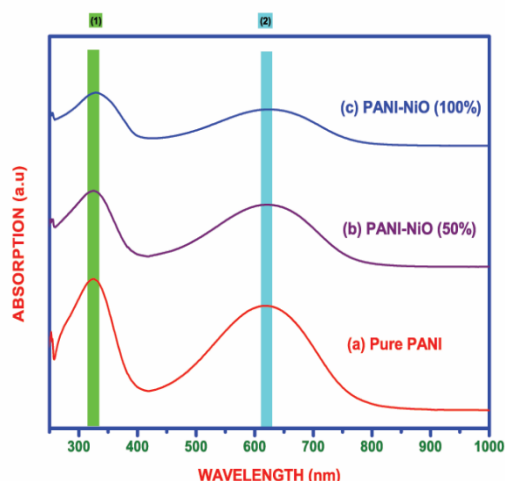
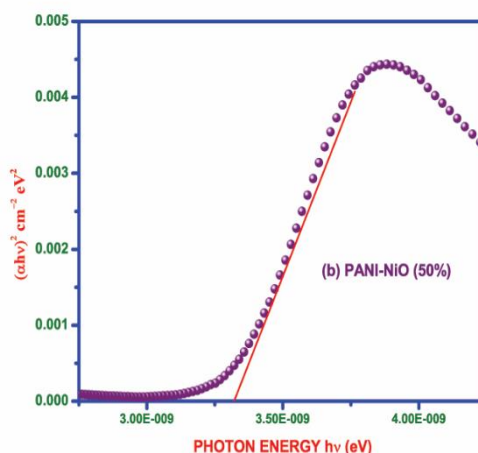
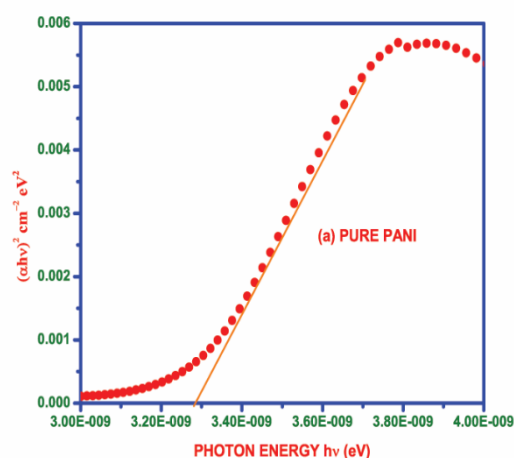


Fig.2 UV-Vis spectra of pure PANI (a) and PANI-NiO (50, 100%) nCs (b) and (c)

This implies that PANI chains and NiO nanoparticles may interact in some way, which could affect the antibacterial properties of the PANI-NiO nanocomposite [27]. NiO nanoparticle surface modification may allow the wavelength of the response light to change from ultraviolet to visible light [28]. When it comes to creating PANI-based conductive nanocomposites, the PANI-NiO nanocomposite is more appropriate and efficient because it demonstrates a good and adjustable suspension property when compared to neat PANI [29]. The band underwent a redshift as well as an intensity decrease; meanwhile, a blueshift and an intensity decrease were noted indicating that, following their interaction with the metal ions [30].

Table.2UV-Vis wavelength and absorption regions of pure PANI and PANI-NiO nCs

Peak No	Parameters	Pure PANI	PANI-NiO (50%)	PANI-NiO (100%)
1	Wavelength	328	323	321
	Absorption	0.67	1.09	2.21
2	Wavelength	627	622	618
	Absorption	0.55	1.00	2.01



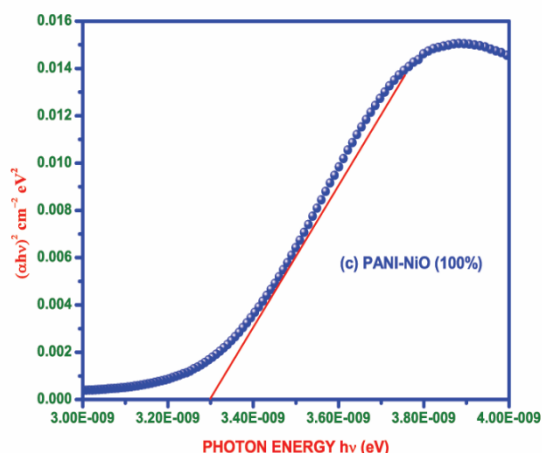


Fig.3 Tauc Plot of pure PANI (a) and PANI-NiO(50, 100%) nCs (b) and (c)

3.3 XRD analysis

Using powder X-ray diffraction (XRD) measurements, the structures of the pure PANI and PANI-NiO nanocomposites and the incorporation of NiO NPs into the PANI moiety were examined. The XRD patterns of the PANI-NiO nanocomposites and pure PANI with varying nanoparticle loading are shown in Fig. 4. The XRD patterns of the pure PANI are shown in Fig. 4a. Pure PANI exhibited broad bands centered at $2\theta = 20.40^\circ$. These bands are attributed to a periodicity perpendicular and parallel to the PANI chains, suggesting that the polymer was created with a low degree of crystallinity [31,32]. A prominent broad peak at $2\theta = 20.40^\circ$ is visible in the spectra of pure PANI (Fig. 4, Pattern a), implying that the produced PANI has a semicrystalline structure.

$$d = \frac{n\lambda}{2 \sin \theta}$$

where θ is the angle between the incident ray and the scattering planes, Cu K α radiation source wavelength is denoted by λ , ($\lambda = 1.5406 \text{ \AA}$), and n is an integer determined by the order given [33]. Using the -Debye-Scherrer equation, the full width at half-maximum (FWHM) at the main peak is typically used to estimate the average grain size.

$$L = \frac{K\lambda}{\beta \cos \theta}$$

where θ is the angle at maximum intensity is denoted by θ , β is the complete width in radians at half maximum is denoted by β , K is a constant at 0.9, and λ is the radiation wavelength is denoted by λ at 1.5148 [34]. PANI-NiO (50%) nanocomposite sample has some sharp peaks centered at $2\theta = 37.24^\circ$ ($d = 2.24 \text{ \AA}$), 43.33°

($d = 2.08 \text{ \AA}$), 62.86° ($d = 1.47$), 75.32° ($d = 1.26$), and 79.35° ($d = 1.20$) which correspond to the Ni planes (111), (200), (220), (311), and (222), respectively. As the nanocomposite was formed, some crystallinity appeared in the polymer matrix, as evidenced by the planes' average crystalline size of 7.12 nm. Although, in the instance of the PANI-NiO (100%) nanocomposite, in addition to the broad peak at 20.4° confirming the polymer chain's existence combined with Ni nanoparticles, peaks at 2θ values of 37.35° ($d = 2.40 \text{ \AA}$), 43.41° ($d = 2.08 \text{ \AA}$), 62.93° ($d = 1.47 \text{ \AA}$), 75.48° ($d = 1.25 \text{ \AA}$), and 79.42° ($d = 1.20 \text{ \AA}$) were observed. These degrees correspond to the (111), (200), (220), (311), and (222) planes of Ni, respectively. 6.40 nm is the typical crystalline size of PANI-NiO (100%). According to XRD, the mean crystalline size of the PANI-NiO nanocomposites ranged from 50% to 100% and decreased as the NiO nanoparticle concentration rose [34]. The peaks widened as the concentration of Ni sources changed, indicating a change in crystallite size. Table.3 shows the tabulated crystalline characteristics of the PANI-NiO nanocomposites. Because PANI is amorphous, no diffraction peaks were observed. Apart from the broad amorphous peak of PANI, distinctive peaks of NiO nanoparticles are apparent in the XRD patterns of the PANI-NiO nanocomposites, indicating that PANI does not change the crystal structure of NiO nanoparticles [35]., the reinforcing substance of NiO nanoparticles and the organic-polymer matrix material of PANI were physically combined [36]. The intensity of the PANI peaks' increased with increasing NiO concentration, suggesting that the inclusion of NiO nanoparticles prevented crystallization of the PANI chains. This implies that PANI and NiO particles in the nanocomposites may interact in some way. It was proposed that there is no chemical interaction between PANI and NiO because the FTIR, UV, or XRD spectra of the PANI-NiO nanocomposites do not show the creation of a new peak.

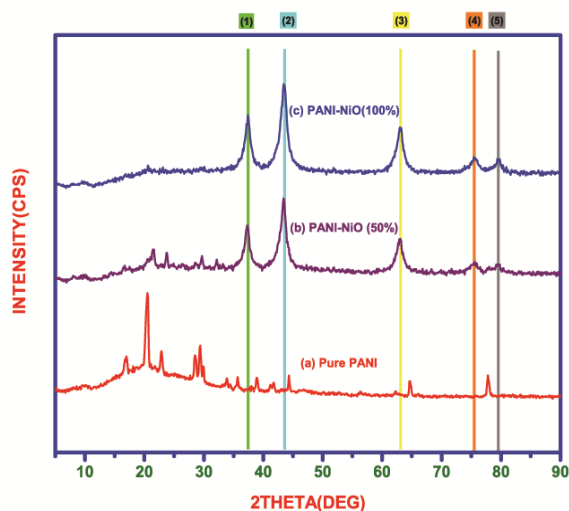


Fig.4 XRD Pattern of pure PANI (a) and PANI-NiO(50%, 100%) nCs (b) and (c)

Table.3Crystalline properties of PANI-NiO (50% &100%) nCs

Peak No	PANI-NiO (50%)										
	2θ (deg)	FWHM (deg)	d spacing Value (Å)	Intensity (Counts)	Crystalline Size (nm)	Dislocation Density $\times 10^{15}$	Strain $\times 10^{-3}$	hkl	Lattice constant a=b=c	Unit cell volume $\times 10^{-28}$	X ray density
1	37.24	1.12	2.24	570	7.47	1.79	6.45	111	4.17	7.29	4.21
2	43.33	1.24	2.08	923	6.84	2.13	6.09	200	4.17	7.26	4.23
3	62.86	1.36	1.47	449	6.83	2.14	4.32	220	4.17	7.29	4.21
4	75.32	1.71	1.26	128	5.83	2.93	4.32	311	4.18	7.31	4.20
5	79.35	1.19	1.20	122	8.67	1.33	2.78	222	4.17	7.30	4.21

Peak No	PANI-NiO (100%)										
	2θ (deg)	FWHM (deg)	d spacing Value (Å)	Intensity (Counts)	Crystalline Size (nm)	Dislocation Density $\times 10^{15}$	Strain $\times 10^{-3}$	hkl	Lattice constant a=b=c	Unit cell volume $\times 10^{-28}$	X ray density
1	37.35	1.39	2.40	676	6.01	2.75	7.98	111	4.16	7.23	4.25
2	43.41	1.43	2.08	1146	5.95	2.82	6.99	200	4.16	7.22	4.25
3	62.93	1.47	1.47	578	6.33	2.49	4.66	220	4.17	7.26	4.23
4	75.48	1.48	1.25	199	6.73	2.20	3.74	311	4.17	7.27	4.22
5	79.42	1.46	1.20	162	7.02	2.02	3.43	222	4.17	7.28	4.22

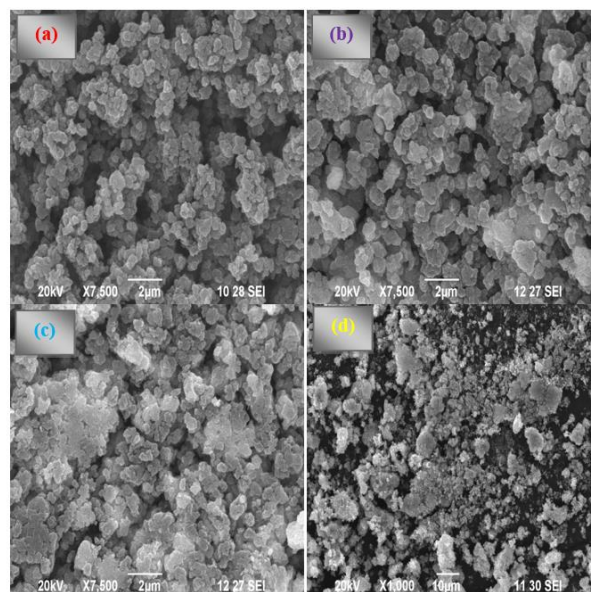


Fig.5 SEM micrographs of pure PANI (a), PANI-NiO (50, 100%) (b, c) nCs and pure Sb_2O_3 (d) nPs

3.4 SEM & EDAX analysis

The morphological alterations that resulted from the interaction of inorganic nanoparticles with the organic polymer matrix are shown in the scanning electron microscopy (SEM) images of the pure PANI and PANI-NiO nanocomposites. The absence of impurity phases is indicated by the binding pattern and consistent surface morphology, as observed in the nanocomposite's SEM image of the nanocomposite. Pure PANI and PANI-NiO nanocomposites with different NiO concentrations were analyzed for surface appearance and structure using SEM. The results are shown in Fig.5. The spherical PANI produced without NiO exhibited uneven stacking. The produced PANI-NiO nanocomposites were completely different from pure irregular spheres. PANI nanoparticles uniformly distributed on Ni nanoparticles were clearly visible in the SEM images of the PANI-NiO nanocomposite with various concentrations of NiO for the two nanocomposites [37]. Furthermore, several spherical PANI agglomerates were observed on the surface of the NiO. The concentration of NiO nanoparticles influenced the morphology of the PANI-NiO nanocomposites. Non-agglomerated, evenly packed PANI was formed on the face of the Ni nanoparticles. From the PANI-NiO nanocomposite, it is evident that the Ni nanoparticles were evenly distributed and fully integrated into the amorphous PANI matrix, and the amount of Ni nanoparticles in the final PANI-

NiO nanocomposite might regulate its shape and structure. Ni nanoparticles were implanted in an amorphous polymer matrix with no features when the Ni concentration was low [38]. EDAX was used to identify the elemental characteristics of the nanocomposites, for various Ni source concentration, as shown in Fig.6. The presence of C, O, S, and Ni in the nanocomposite indicates the presence of NiO and PANI. A summary of these findings for the elemental composition of the PANI-NiO nanocomposites is shown in Table.4. The EDAX method for analyzing the sample composition revealed that the spectrum of characteristic X-ray radiation arising from the interaction of an electron probe with the sample surface contains peaks representing chemical elements that contribute to the formation of PANI-NiO nanocomposites (C, O, S and Ni) and pure PANI (only C, O, and S).

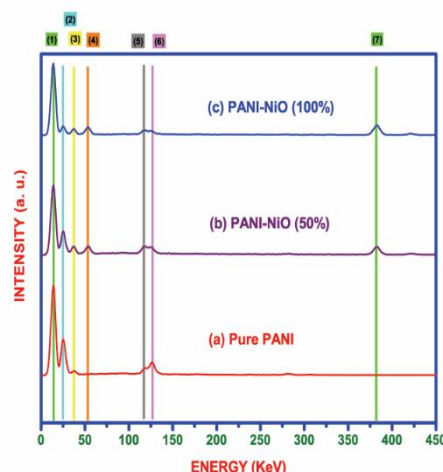


Fig.6 EDAX Spectrum of pure PANI (a), PANI-NiO (50, 100%) (b, c) nCs

Table.4 Chemical composition of pure PANI and PANI-NiO nCs

Element	Weight (%)		
	Pure PANI	PANI-NiO (50%)	PANI-NiO (100%)
Carbon	84.05	59.34	45.17
Oxygen	11.45	23.21	23.35
Sulfur	4.50	1.28	0.72
Nickel	-	16.16	30.76

The components concentration are that make up the nanocomposite, which was made via a mechanical mixing process. With a certain degree of precision, judgments regarding the molecular makeup of the sample can be drawn from the study of this table [39].

3.5 TGA & DSC analysis

TGA was employed to examine the material stability at high temperatures, and Fig.7 compares the mass losses that occurred from heating pure PANI and the PANI-NiO nanocomposites in a nitrogen environment. An unstable mass drop was observed in the pure PANI (Fig.7a) at temperatures between 75 °C - 150 °C, 250 °C -300 °C, and above 500 °C; water molecules were ejected from the polymer structure at low temperatures, and either the breakdown of the polyaniline chain skeleton after the dopant was removed from the polymer structure or the release of an acid dopant bound to the polyaniline chain could be the cause of the decreased weight at higher temperatures [40]. However, in the case of the PANI-NiO nanocomposites (Fig.7b and c), a gradual mass drop was observed at 450 °C. However, at temperatures lower than 450 °C, however, there was a sudden change in mass. The total residual mass losses up to 600 °C for pure PANI and PANI-NiO nanocomposites of 50% and 100%, respectively, were approximately 35.81, 49.84, and 54.65% are respectively, and the data show that the capping of nickel nanoparticles within the PANI matrix confirms the improved trend of the degradation curve for PANI-NiO nanocomposites [41]. The increased heat resistance in the PANI-NiO polymer nanocomposites is due to the strong interactions between the metal oxide nanoparticles and the polymer matrix. The initial estimation of particle loading based on the initial weights of the polymers and nanoparticles was significantly smaller than that of the polymer nanocomposites [42]. The incomplete conversion of the PANI is the cause of this. The slight variance in residue between the polymer

nanocomposites is attributed to the chemical impact left by the metal oxide nanoparticles on the processing of the nanocomposites.

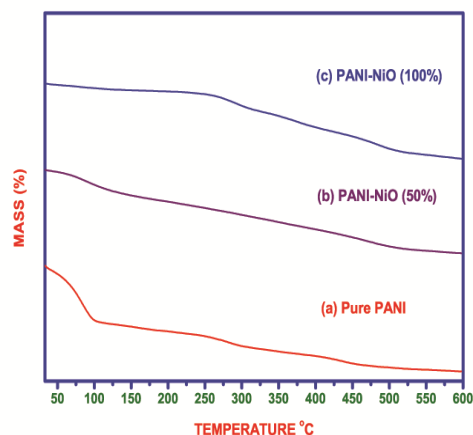


Fig.7 TGA spectrum of pure PANI (a), PANI-NiO (50, 100%) (b,c) nCs

A greater degree of thermal stability is seen following polymer development over NiO [43]. Decomposition of polymer nanocomposites typically results in a two-step weight loss. The first stage may indicate the loss of a polymer's side chain, while the second step can indicate the polymer's backbone burning. Additional details regarding the thermal characteristics of pure PANI and its PANI-NiO nanocomposites can be obtained using DSC measurement. Our PANI-NiO nanocomposite has great thermal stability, as demonstrated in Fig. 8 DSC findings, and it is appropriate to be employed in medical applications [44]. Conversely, the melting temperature of PANI in the polymer nanocomposites is significantly influenced by the nanoparticles. According to the XRD investigation [45], the addition of NiO to PANI causes its crystalline structure to become less pronounced, which results in a decreased melting temperature of PANI in the nanocomposites with a higher particle loading. The breakdown temperature of polymer nanocomposites containing varying weight percentages of NiO nanoparticles is nearly constant, but the thermal stability of these composites varies. Compared to pure PANI, the ability to endure heat of polymer nanocomposite materials was enhanced by the inclusion of NiO nanoparticles. [46].

Compared to pure PANI, the PANI-NiO nanocomposites show a lower beginning decomposition temperature. This is linked to the release of moisture and organic solvent residue that becomes entangled in the PANI polymer chains. The limited breakdown function of the nanocomposites and the protective effect of the

Table.5 Weight loss and residual mass of pure PANI and PANI-NiOnCs

Sample Name	Mass Changes	Residual Mass (%)
Pure PANI	Stage: 1	-35.89
	Stage: 2	-16.34
	Stage: 3	-11.96
	Stage: 4	-
	Residual Mass	-35.81
	Residual Temperature	597 °C
PANI-NiO (50%)	Stage: 1	-18.72
	Stage: 2	-14.27
	Stage: 3	-17.17
	Stage: 4	-
	Residual Mass	-49.84
	Residual Temperature	597 °C
PANI-NiO (100%)	Stage: 1	-5.19
	Stage: 2	-12.00
	Stage: 3	-10.59
	Stage: 4	-17.57
	Residual Mass	-54.65
	Residual Temperature	597 °C

NiOnanoparticles are linked to the processes of the increased heat stability [47].

3.6 Antibacterial activity

The antibacterial activity of the materials was investigated using the powder inhibition zone, least inhibitory concentration, and minimal bactericidal concentration methods against *Escherichia coli* and *Staphylococcus aureus*.

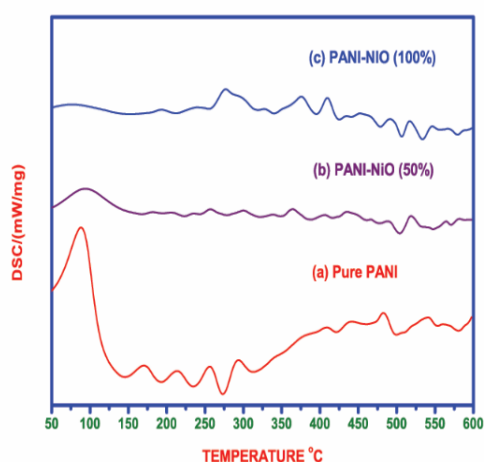


Fig.8 DSC spectrum of pure PANI (a), PANI-NiO (50, 100%) (b,c) nCs

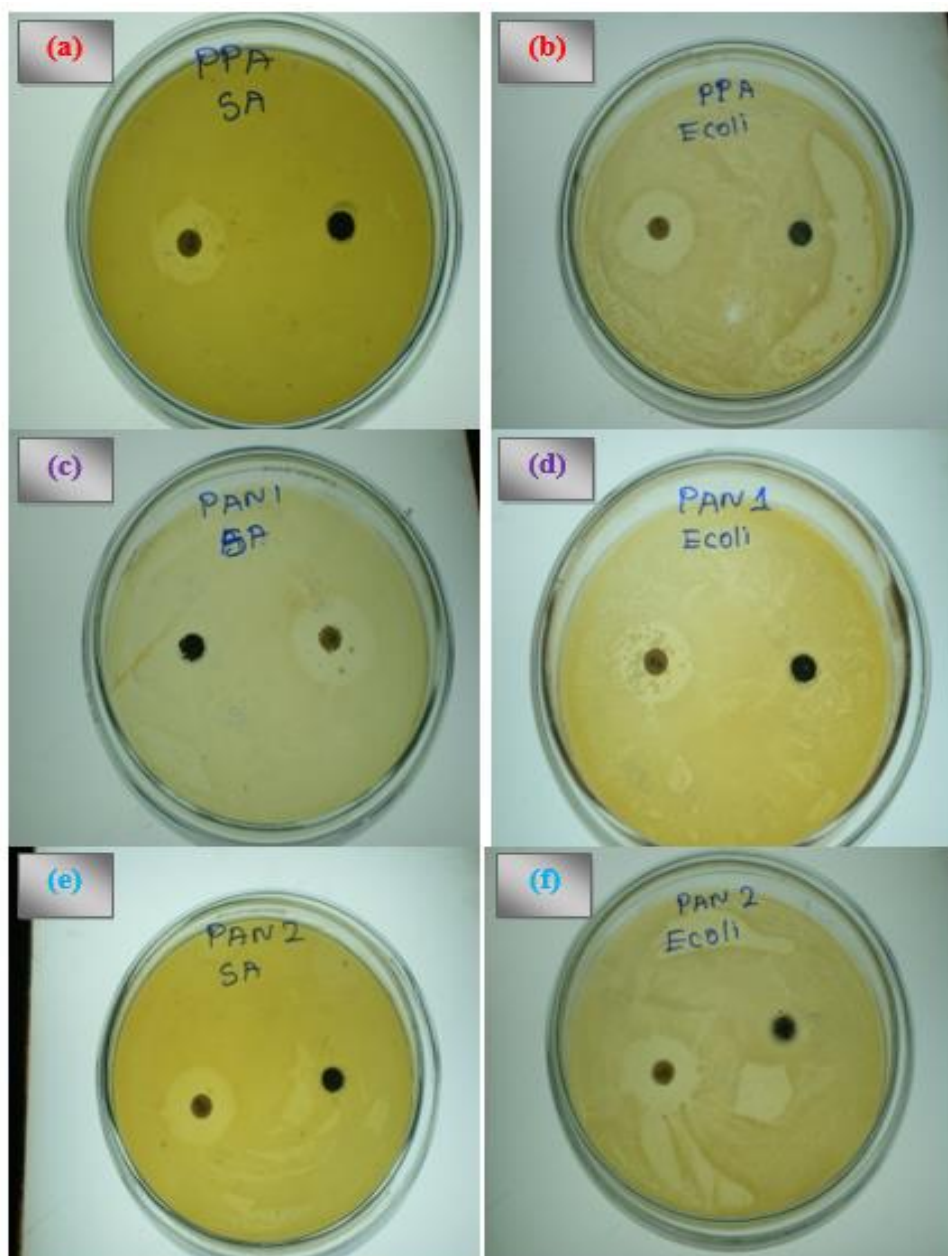


Fig.9 Antibacterial activity photograph of pure PANI and PANI-NiO (50%, 100%) nCs, pure PANI (a) *Staphylococcus aureus* (b) *E. coli*, PANI-NiO (50%) (c) *Staphylococcus aureus* (d) *E. coli* and PANI-NiO (100%) (e) *Staphylococcus aureus* (f) *E. coli*

These results unequivocally demonstrate that PANI-NiO nanocomposites have outstanding antibacterial activity against the growth of germs. Table 6 lists the antibacterial properties of the PANI-NiO nanocomposites and pure PANI. *E. coli* exhibited superior antibacterial activity compared to pure PANI, while PANI-NiO nanocomposites, at 50% and 100%, exhibited a wide range of antibacterial activity against *S. aureus*. Additionally, the NiO content of the PANI-NiO nanocomposites enhanced their antibacterial activity. *S. aureus* and *E. coli* were observed in the PANI-NiO nanocomposites. In

terms of resistance to antibiotic agents, *E. coli* has a considerable advantage over other bacterial strains because of its distinct cell membrane structure. The zones of inhibition for each sample are presented in Table.6 for quantitative comparison. The bactericidal and bacteriostatic activities of the PANI-NiO nanocomposites were superior to those of pure PANI. Fig. 9 [48] displays images of the antibacterial activities of the pure PANI and PANI-NiO nanocomposites.



Table.6 Zone of inhibition value of pure PANI and PANI-NiO nCs

Samples	Zone of Inhibition (mm)	
	E coli	Staphylococcus aureus
Pure PANI	11±0.4	6±0.8
PANI-NiO (50%)	13±0.9	8±0.9
PANI-NiO (100%)	16±0.6	11±0.5

4. Conclusion

The list of innovative materials and nanocomposites includes conducting polymer nanocomposites, which are highly significant. Several techniques, including FTIR, UV-Vis, XRD, SEM, and EDAX, as well as antibacterial activity, are used to completely analyze the morphology and structure of these nanocomposites and the pure PANI, PANI-NiO nanocomposites. A PANI-NiO hybrid nanocomposites material was in due course the NiO nanoparticles being enclosed in the expanding polymer chains, according to the molecular structure characterizations of the PANI-NiO nanocomposites. The findings show that the presence of NiO nanoparticles in the PANI nanocomposite dramatically altered the optical properties of the PANI-NiO nanocomposite, including absorbance, peak intensity, and band gap. The PANI-NiO nanocomposites' crystalline and cubic structure, as well as their 50% and 100% crystalline sizes of 7.12 nm and 6.40 nm, respectively, were amply demonstrated by XRD investigations. The finding of a change in the lattice characteristics of NiO in the PANI-NiO nanocomposites is further supported by the SEM images, which show an interaction between the PANI matrix and NiO nanoparticles. The H₂SO₄ doped PANI-NiO nanocomposite underwent morphological investigation using SEM, which showed the formation of a spherical surface. According to the TGA profiles, addition of NiO nanoparticles considerably increased the thermal stability of the PANI-NiO nanocomposites. In comparison to the residual mass of pure PANI (35.81), extended thermal investigation shows that the residual mass of these nanocomposites varies by 49.84 (50%), 54.65 (100%). The higher residual mass of the nanocomposites indicates a stronger bonding degree between NiO and PANI as well as a higher thermal stability. These polymer nanocomposites also have the advantages of good surface shape and elemental composition. Further research will consider the synthesis of nanocomposites using different metal concentrations of NiO inside the polymer matrix

in the mechanical mixing method of these experimental results to assess the possibility of tuning and possibly enhancing the related physical chemistry properties. The resulting nanocomposites also displayed antibacterial reagent behaviour and the PANI-NiO nanocomposite emeraldine base composition seems to be crucial for improving the medical field performance. Therefore, the PANI-NiO nanocomposite exhibited strong antibacterial activity, which is recommended for various therapeutic applications. Additional conducting PANI nanocomposites with various metal oxide concentrations and compositions were prepared this study.

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References

- [1] Jui-Ming Yeh, Shir-Joe Liou, Chiung-Yu Lai and Pei-Chi Wu, Chem. Mater **13** (1) 1131 (2001).
- [2] Rupali Gangopadhyay and Amitabha De, Chem. Mater **12** (7), 608 (2000).
- [3] Luiz C. Mariano, Rodrigo V. Salvatierra, Carlos E. Cava, Marlus Koehler, Aldo J. G. Zarbin and Lucimara S. Roman, J. Phys. Chem. C **118** (43), 24811(2014).
- [4] Hua Zou, Shishan Wu and Jian Shen, Chem. Rev **108** (9) 3893 (2008).
- [5] Lei Wang, Melissa Rocci-Lane, Paul Brazis, Carl R. Kannewurf, Young-Il Kim, Woo Lee, Jin-Ho Choy and Mercuri G Kanatzidis, J. Am. Chem. Soc **122**, 6629 (2000).



- [6] Sunil K. Pillalamarri, Frank D. Blum and Massimo F. Bertino, *Chem. Commun* **1** (36), 4584 (2005).
- [7] Li Wang, Xingping Lu, Shengbin Lei and Yonghai Song, *J. Mater. Chem. A* **2** (13) 4491 (2014).
- [8] Bin Zhang, Botao Zhao, Shenghui Huang, Ruiying Zhang, Ping Xu and Hsing-Lin Wang, *Cryst Eng Comm* **14** (5), 1542 (2012).
- [9] Bhagwati Sharma, Sonam Mandani and Tridib K. Sarma, *J. Mater. Chem. B* **2** (26) 4072 (2014).
- [10] Hangjun Ding, Xian-Ming Liu, Meixiang Wan and Shao-Yun Fu, *J. Phys. Chem. B* **112** (31), 9289 (2008).
- [11] Xinxing Zhang, Xiaodong Wu, Canhui Lu and Zehang Zhou, *Chem. Eng* **3** (4), 675 (2015).
- [12] Md. Dilwar Alam Khan, Arshia Akhtar, Syed Ashfaq Nabi and Meraj Alam Khan, *Ind. Eng. Chem. Res* **53** (39), 15253 (2014).
- [13] Yu Qiu and Lian Gao, *J. Phys. Chem. B* **109** (42) 19732 (2005).
- [14] Jose J. Alcaraz-Espinoza, Alicia E. Chavez-Guajardo, Juan C. Medina-Llamas, Cesar A. S. Andrade and Celso P. de Melo, *ACS Appl. Mater. Interfaces* **7** (13) 7231 (2015).
- [15] Wei Feng, Xiaojun Zhou, Wei Nie, Liang Chen, Kexin Qiu, Yanzhong Zhang and Chuanglong He, *ACS Appl. Mater. Interfaces* **7** (7), 4354 (2015).
- [16] Anna Drury, Shweta Chaure, Michael Kroll, Valeria Nicolosi, Nandu Chaure and Werner J. Blau, *Chem. Mater.* **19** (17) 4252 (2007).
- [17] Zhidan Lin, Zixian Guan and Zhuoyao Huang, *Ind. Eng. Chem. Res* **52** (8), 2869 (2013).
- [18] Guofa Cai, Jiangping Tu, Ding Zhou, Jiaheng Zhang, Qinqin Xiong, Xuyang Zhao, Xiuli Wang and Changdong Gu, *J. Phys. Chem. C* **117** (31) 15967 (2013).
- [19] Marcela M. Oliveira, Eryza G. Castro, Carla D. Canestraro, Daniela Zanchet, Daniel Ugarte, Lucimara S. Roman and Aldo J. G. Zarbin, *J. Phys. Chem. B* **110** (34) 17063 (2006).
- [20] Gordana Ciric, Marjanovic, Vera Dondur, Maja Milojevic, Milos Mojovic, Slavko Mentus, Aleksandra Radulovic, Zorica Vukovic and Jaroslav Stejskal, *Langmuir* **25** (5), 3122 (2009).
- [21] Yu Gao, Decai Shan, Fei Cao, Jian Gong, Xia Li, Hui-yan Ma, Zhong-min Su and Lun-yu Qu, *J. Phys. Chem. C* **113** (34) 15175 (2009).
- [22] Xiaorong Gan, Huimin Zhao, Shuo Chen, Hongtao Yu and XieQuan, *Anal. Chem.* **87** (11), 5605 (2015).
- [23] Hesheng Xia and Qi Wang, *Chem. Mater.* **14** (5), 2158 (2002).
- [24] Dan Ping Wang and Hua Chun Zeng, *Chem. Mater* **21** (20) 4811 (2009).
- [25] Antonio F. Frau, Thomas J. Lane, Andrea E. Schlather, Jin Young Park and Rigoberto C. Advincula, *Ind. Eng. Chem. Res.* **50** (9) 5532 (2011).
- [26] Celly M. S. Izumi, Gustavo F. S. Andrade and Marcia L. A. Temperini, *J. Phys. Chem. B* **112** (51) 16334 (2008).
- [27] Tao Guo, Lishi Wang, David G. Evans and Wensheng Yang, *J. Phys. Chem. C* **114** (11), 4765 (2010).
- [28] Dmitri Yu. Godovskya Andrei E. Varfolomeev, David F. Zaretsky, R. L. Nayana Chandrakanthi, Andreas Kundig, Christoph Weder and Walter Caseri, *J. Mater. Chem* **11** 2465 (2001).
- [29] Dongjie Li, Yu Li, YiyuFeng, Wenping Hu and Wei Feng, *J. Mater. Chem. A*, **3** (5) 2135 (2015).
- [30] Fan Zhang, Huaqiang Cao, Dongmei Yue, Jingxian Zhang and Meizhen Qu, *Inorg. Chem* **51** (17), 9544 (2012).
- [31] Lorena M. A. Monzon, Karsten Rode, M. Venkatesan, and J.M.D. Coey, *Chem. Mater* **24** (20), 3878 (2012).
- [32] Kai Zhang, Li Li Zhang, X. S. Zhao and Jishan Wu, *Chem. Mater.* **22** (4) 1392 (2010).
- [33] Vipin Kumar and Pooi See Lee, *J. Phys. Chem. C* **119** (17), 9041 (2015).
- [34] Lirong Kong, Xiaofeng Lu, Xiujie Bian, Wanjin Zhang and Ce Wang, *ACS Applied Materials and Interface* **3** (1), 35 (2011).
- [35] Lu Wang, Lin Chen, Bo Yan, Chunguang Wang, Feng Zhu, Xuefan Jiang, Yimin Chao and Gang Yang, *J. Mater. Chem. A* **2** (22) 8334 (2014).
- [36] D. Damodara, R. Arundhathi and Pravin R. Likhar, *Catal. Sci. Technol* **3**, 797 (2013).
- [37] Guiheng Xu, Nan Wang, Junyi Wei, Leilei Lv, Jianan Zhang, Zhimin Chen, and Qun Xu, *Ind. Eng. Chem. Res.* **51** (44), 14390 (2012).
- [38] Saptarshi Dhibar and Chapal Kumar Das, *Ind. Eng. Chem. Res* **53** (9), 3495 (2014).
- [39] Wen Yuan, Hui Zhao, Heyi Hu, Shen Wang and Gregory L. Baker, *ACS Appl. Mater. Interfaces* **5** (10), 4155 (2013).
- [40] Rodrigo V. Salvatierra, Marcela M. Oliveira and Aldo J. G. Zarbin, *Chem. Mater* **22** (18), 5222 (2010).
- [41] Pallavi Mavinakuli, Suying Wei, Qiang Wang, Amar B. Karki, Sanjay Dhage, Zhe Wang, David P. Young and Zhanhu Guo, *J. Phys. Chem. C* **114** (9), 3874 (2010).
- [42] Devasish Chowdhury, *J. Phys. Chem. C*, **115** (28), 13554 (2011).
- [43] Lakshinandan Goswami, Neelotpal Sen Sarma, and Devasish Chowdhury, *J. Phys. Chem. C* **115** (40), 19668 (2011).
- [44] Wu Chun-Guey, Hwang Jiunn-Yih and Hsu Shui-Sheng, *J. Mater. Chem* **11** (8), 2061 (2001).
- [45] Jiahua Zhu, Suying Wei, Lei Zhang, Yuanbing Mao, Jongeun Ryu, Neel Haldolaarachchige, David P. Young and Zhanhu Guo, *J. Mater. Chem* **21** (11), 3952 (2011).
- [46] Xi Zhang, Qingliang He, Hongbo Gu, Suying Wei and Zhanhu Guo, *J. Mater. Chem. C* **1** (16), 2886 (2013).
- [47] Xiaoxi Liang, Mengxi Sun, Liangchao Li, Ru Qiao, Keyu Chen, Qiushi Xiao and Feng Xu, *Dalton Trans* **41** (9), 2804 (2012).