

Optical and Photocatalytic Activity of Polyaniline/TiO₂ Composites with Anatase and P25 Nanoparticles

M.M. Zahornyi^{1,*}, N.I. Tyschenko¹, A.V. Ragulya¹, O.M. Lavrynenko¹, A.M. Kasumov¹,
A.K. Melnyk^{2,†}, O.V. Kuzma^{3,‡}, A.I. Ievtushenko¹

¹ Institute for Problems of Materials Science, 3, Krzhyzhaniivskoho St., 03142 Kyiv, Ukraine

² Institute for Sorption and Problems of Endoecology, 13, General Naumov St., 03164 Kyiv, Ukraine

³ National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37, prosp. Peremohy, 03056 Kyiv, Ukraine

(Received 11 August 2021; revised manuscript received 20 October 2021; published online 25 October 2021)

In the present paper, polyaniline (PANI) has been successfully synthesized on the surface of TiO₂ nanoparticles of different nature. The morphology, particle size, optical activity and photocatalytic performance of the obtained materials were systematically studied by various analytical techniques. Ultraviolet-visible (UV-Vis), EPR characterizations of PANI-TiO₂ nanocomposites confirmed interactions between the polymer and TiO₂ nanoparticles. The EPR results show that nanocomposite sample m1, in which PANI retains a more ordered structure, can be preferred for use as a photocatalyst. Photocatalytic properties of PANI-TiO₂ nanocomposites were examined by degradation of phenol with a concentration of 50 mg l⁻¹ under UV light irradiation. The results showed that phenol degradation occurs maximally during the first 10 min for systems with P25 in comparison with anatase systems. The maximum value of V is 4.50 %/min for sample m1 (PANI-TiO₂-P25). Due to the synergistic effect between PANI and TiO₂, it is capable of absorbing visible light more efficiently and decreasing the process of electron-hole recombination. It was stated that the polyaniline film is a good sensitizer after UV irradiation. The excellent photocatalytic effect of PANI-TiO₂ is attributed to the synergistic effect between PANI and TiO₂ which promotes the migration efficiency of the photogenerated carriers at the PANI-TiO₂ interface (EPR). Mathematical analysis illustrates the rate of phenol degradation by the curves with fourth and sixth order polynomials.

Keywords: Photocatalyst, TiO₂, Anatase, Polyaniline, Hole, UV-Vis, Nanocomposite, Irradiation.

DOI: [10.21272/jnep.13\(5\).05034](https://doi.org/10.21272/jnep.13(5).05034)

PACS numbers: 32.30.Rj, 33.20.Lg, 42.62.Fi, 61.46. – W, 77.22. – d

1. INTRODUCTION

Photocatalytic degradation is an efficient and economical method that has attracted increasing attention because it is particularly useful for cleaning biologically toxic or non-degradable materials such as aromatics, pesticides, petroleum constituents, and volatile organic compounds in wastewater [1-3]. The contaminant materials are converted to a large extent into stable inorganic compounds such as water, carbon dioxide, and salts, i.e., they undergo mineralization [3]. In previous publications, it has been shown that TiO₂ is an excellent photocatalyst due to high chemical stability and photocatalytic activity [4-6]. But TiO₂ has a wide band gap (3.2 eV), which restricts its use to UV light, which occupies only 3-5 % of solar energy utilization [5]. So, it is important to modify the optical response of TiO₂ from UV to a visible light range by shortening its band gap. Recently, a conducting polymer has shown great potential as a photosensitizer under UV irradiation due to its narrow band gap and π - π^* transition, in which an electron can be excited from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) [7-8]. The study [9] was undertaken to evaluate the degradation of phenol and p-cresol as recalcitrant aromatic compounds in abattoir wastewater using TiO₂/ZnO composite doped with polyaniline (PANI). Detergents and residual blood were the main

sources of organic matter in wastewater. The method used to prepare the composite was *in situ* chemical oxidative polymerization of aniline and was tested in a ring reactor equipped with a 25W UV-C lamp. Xu et al. found that the photocatalytic activity of the hierarchical rutile TiO₂ nanorods spheres was about twice that of the famous commercial photocatalyst P25 [10]. However, hierarchical rutile TiO₂ nanorods spheres do not use visible light. To get a material with high visible light photocatalytic activity, a novel PANI-TiO₂ nanocomposite with bionic nanostructure was synthesized by a facile hydrothermal method in the work. Although TiO₂ photocatalytic activity under Vis (> 400 nm) can be increased by doping; and numerous groups utilize metal ions, such as Fe, Au, Ag, V, Cr, Sn, C-S to hinder the recombination process [11-14]. The recombination process in TiO₂ has also been suppressed by preparing PANI/TiO₂ composites, which is promising, though poorly investigated approach. The advantage is that PANI is a conductive, non-toxic, and thermally stable polymer with a high absorption coefficient in the Vis spectrum. The absorbance in the UV-Vis spectra is observed to increase in the whole range of UV-Vis wavelengths with the increase in the concentration of TiO₂ in PANI-TiO₂ nanocomposites.

Thus, it is important to create a composite photo-generator based on TiO₂ to control the distribution of h⁺ (generation) and subsequent use for the effective

* mzahornyi81@gmail.com
mak106@ukr.net
olekuz6@gmail.com

destruction of toxic compounds due to the high concentration of oxide radicals. The aim of the present work is to test the effects of TiO₂ morphological properties of *in situ* prepared TiO₂/PANI samples with monomer concentration on the photocatalytic activity in the reaction with phenol.

2. EXPERIMENTAL

Hydrochloride aniline (HAn) monomer (purity 98 %), ammonium persulfate (APS) as oxidizer (Merk), TiO₂ anatase (Aldrich Sigma), P25 “Evonic” particles 20 nm in size, deionized water, hydrochloric acid, ethanol (Aldrich Sigma) were used as received without purification. PANI/TiO₂ composites were formed by *in situ* polymerization method. First, nanoparticles of TiO₂ were modified by water solution of HAn, using homogenizer ULAB2200 (Germany) at a speed of 300 min⁻¹ for 1 h. Then, the APS solution was added dropwise at 0 °C. Polymerization on the surface of oxide nanoparticles was carried out at a pH of 2-4. The *in-situ* polymerization process resulted in a dark green product. After that, the obtained nanocomposites were washed with deionized water, acetone, ethanol, respectively. Then, PANI/TiO₂ nanocomposites were dried at 50 °C for 24 h. PANI was synthesized according to technique in [7] using oxidative radical polymerization at 0 °C. The samples were characterized by TEM (JEOL JEM-1400), UV-Vis absorption spectra “Cary” 300 Scan, UV-Vis-NIR spectrophotometer, Australia. EPR spectra of TiO₂, PANI, PANI-TiO₂ were recorded on an X-band spectrometer Bruker Eleksys E580 at a temperature of 298 K, the conditions for recording spectra were as follows: frequency 9.38 GHz, microwave power 2 mW, modulation intensity from 0.1 to 1 G at modulation frequency 100 kHz, scanning width 100 G, resolution 1024 points. A sample of diphenylpicrylhydrazyl ($g = 2.0036$) was used for the spectrometer calibration.

The photocatalytic activity of PANI-TiO₂ were evaluated in the degradation of model phenol compound. A 300 W Xe lamp was used as a light source. The photocatalytic degradation of phenol was measured at ambient pressure and room temperature in a photoreactor set up. An aqueous solution of phenol with an initial concentration C_0 of 50 mg l⁻¹ was mixed with prepared nanocomposite powder. Before irradiation, the suspension was left in dark for 30 min to achieve adsorption-desorption equilibrium between the photocatalyst and phenol. The photocatalytic reaction was then started by irradiating the suspension with a lamp. Air was supplied to the suspension during adsorption-desorption and irradiation of light. Then, 0.5 ml of the phenol suspension was withdrawn at regular time intervals and centrifuged at a speed of 10 rpm. The concentration of remaining phenol was analyzed using a UV-visible spectrometer, and the percentage of degradation was calculated.

The degradation rate of phenol V (%/min) was calculated using the equation:

$$V = \frac{C_0 - C}{C_0} \frac{1}{t} 100\%,$$

where C_0 is the initial concentration of phenol.

Interpolation polynomials $P_n(t)$ for experimental concentrations $C(t_k)/C_0$, $k = 0, 1, \dots, n$, will be constructed in the fourth section in Newtonian form for $n = 4$ and $t_k = 0, 10, 20, 30, 40$ min of UV action (and for $n = 6$ in the final case) and corresponding curves there will be shown.

3. RESULTS AND DISCUSSION

Earlier results showed that with increasing concentration of the oxidizer to the monomer in the polymer medium, the yield and doping degree decrease, and the residual monomer content increases. This may be due to peroxidation of the polymer due to the formation of aniline oligomers in the synthesis of the polymer, which can wet the surface, breaking the chain of conjugation. In the acid environment of the polymer, the yield is greater than 80 %. SEM showed that PANI powder at a ratio Ox/An = 1.25 has a developed surface structure and consists of nanoparticles with an average pore size of 10-14 nm in comparison with a sample with Ox/An = 1.0, 3.0. Thus, we concluded that the ratio Ox/An = 1.25 was optimal for the synthesis and characteristics of PANI [7]. So, this ratio was used to synthesize PANI composites with a different nature of TiO₂. Conditions, component concentrations and parameters of the polymerization process are presented in Table 1.

Table 1 – Composition of the reaction mixture and parameters of the polymerization process

N_0	Sample	Quantity monomer, g	pH	t , min (green color)
1	TiO ₂	–	–	–
2	P25	–	–	–
3	k1	0.025	2.45	20
4	m1	0.025	3.20	30

Notice: k1 – polyaniline with TiO₂ (Aldrich), m1 – polyaniline with TiO₂P25 (Evonic)

We assume that the surface of nanosized TiO₂ influences the decomposition of the oxidizing agent. In this case, free radicals are formed on the surface of TiO₂ nanoparticles. The monomer is adsorbed on the surface of nanoparticles, forming groups of activated molecules at a very low polymerization temperature. Also, there are protons of hydroxyl groups on the surface of TiO₂ because the polymerization is carried out in an acidic medium.

For anatase, intense absorption bands are in the short-wavelength UV region (Fig. 2). For a pure conductive polymer, there are two intense bands in the visible region of 550-600 nm (the polymer has conjugated bonds). The absorption band at 402-420 nm is due to polaron- π^* transition in PANI [7].

When adding a polymer of lower concentration, the absorption band was wider compared to pure TiO₂ and polymer. We see the physicochemical interaction between TiO₂ and polymer. Anatase TiO₂ can absorb light with wavelengths below 400 nm. Pure PANI presents characteristic bands at 350-415 and 550-600 nm, which are attributed to the π - π^* transition of the benzenoid ring and π -polaron excitation transition of the quinonoid ring, respectively. So, doped PANI also has high ab-

sorption in the visible-light region. For the composite sample k1, we observed three absorption bands at 250-300 nm, 350-500 nm and 550-750 nm in comparison with the spectra of [7]. There may be a strong π - π^* transition of the benzenoid ring and an interaction between TiO₂ and doped PANI. This is possible because of charge carrier delocalization due to the conformation of the extended PANI chain. PANI-TiO₂ nanocomposites produce more electron-hole pairs under light illumination, and this is expected to increase the photocatalytic activity.

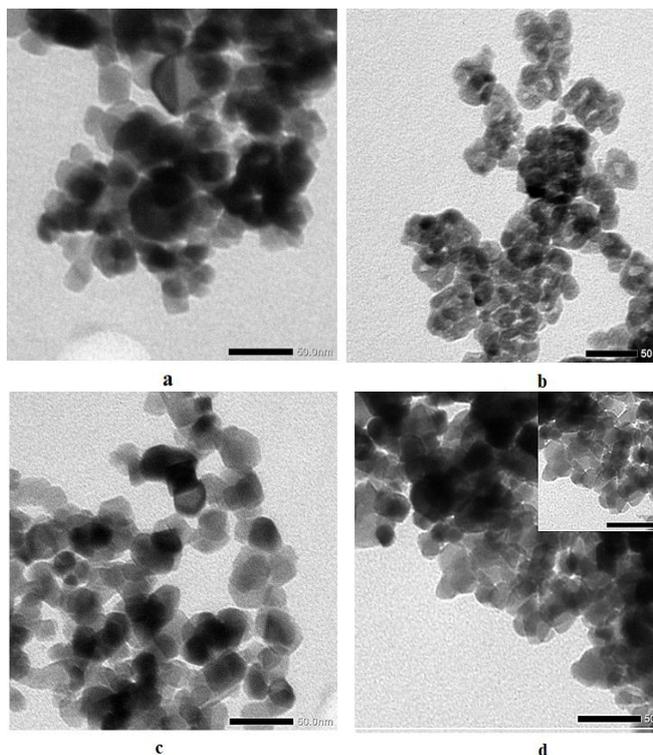


Fig. 1 – TEM images of polymer/TiO₂ (a) anatase, (b) k1, (c) P25, (d) m1. Scale 50 nm

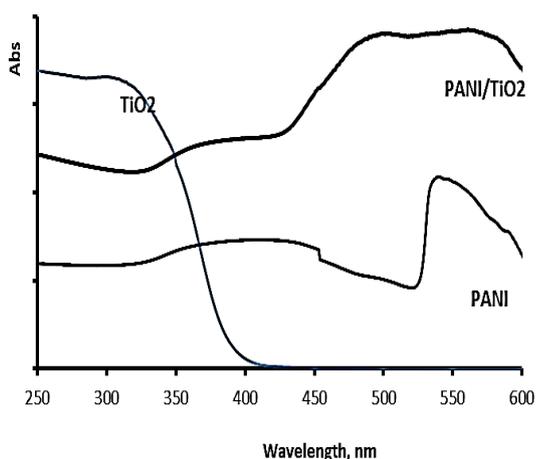


Fig. 2 – UV-Vis spectra of TiO₂, PANI, and k1 samples

Investigations of the initial samples of titanium dioxide nanopowders by EPR spectroscopy showed the presence of relatively weak signals in the range of g -factor values of 1.99-2.00 (Fig. 3). Some authors assign such signals to lattice electron trapping states or to

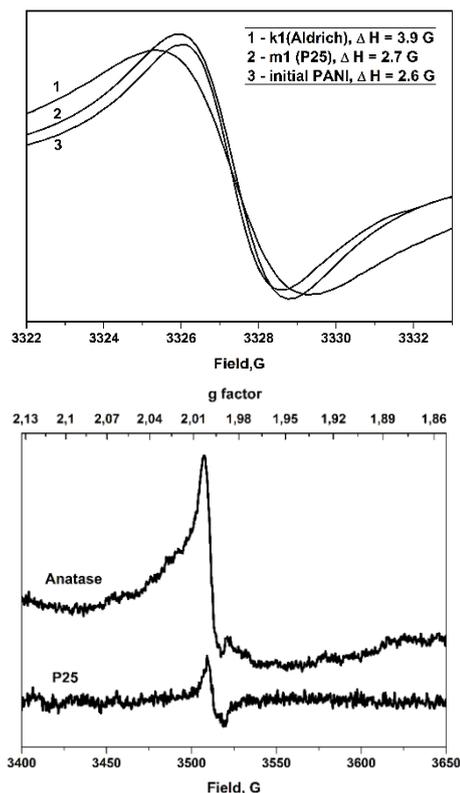


Fig. 3 – EPR spectra of TiO₂, PANI/TiO₂ and PANI samples

surface hole trapping states [20]. In [21], the EPR spectra of TiO₂- x -T anatase nanoparticles show similar lines with a g value of 1.99, which the authors attribute to Ti³⁺ ions in anatase, assuming that free electrons occupy the internal Ti position which leads to the formation of Ti³⁺ defects. The experimental data show that the concentration of paramagnetic centers is significantly higher for anatase nanoparticles; in this case, the absence of a resolved structure of the spectra for both samples, as well as relatively wide lines, may indicate the formation of PMC nanoclusters. It can also be assumed that there are two types of centers in the case of anatase nanoparticles. Studies at a temperature of liquid nitrogen (77 K) did not reveal any significant concentration of trivalent titanium ions ($g = 1.94$ - 1.95). The EPR spectra of both the initial PANI and two composites (Fig. 3) show strong singlet lines with a shape close to Lorentzian, and the g factor values were typical for doped PANI (2.0027-2.0028), corresponding to delocalized conducting electrons. Since signals of the initial samples of nanoparticles were 2-3 orders of magnitude weaker, they did not produce a serious observable contribution to the resulting spectra of the composites.

For all three investigated samples (initial PANI and two composites), EPR spectral lines were practically symmetrical and did not show asymmetry typical for Dysonian lines. An analysis of the line widths shows that for the P25-based composite, broadening is practically absent in comparison with the initial PANI, while for the anatase-based composite it is quite significant. Some authors proposed a model of two-component spectra with close values of g and different linewidths for such binary systems [22, 23]. A narrow one may belong to ordered (isolated) regions of PANI chains (quasi-one-

dimensional morphology) with paramagnetic species with relatively fast motions, such spin diffusion contributes to the motional averaging effect. A broader line can be produced by polarons involved in homogenous disordered media (1D or 3D) or inhomogeneous disorder. Thus, the difference in the width and intensity of spectral lines for the spectra of composites recorded at room temperature (295 K) with different TiO₂ can be determined both by the nature of TiO₂ and, on the other hand, by the surface morphology and size of TiO₂ nanoparticles. Such factors can affect the interaction of charge carriers with lattice optical phonons of PANI chains, and also the dipole-dipole interactions between spins, leading to a change in the exchange of the EPR line. The authors of [7, 15] explained the response-enhancing phenomenon of EPR signal increase in the case of TiO₂/PANI composites by efficient charge separation, which also influences the photocatalytic activity. Synthesized PANI/anatase and PANI/P25 with monomer content were exposed to UV. The results of UV irradiation showed that faster phenol degradation occurs during the first 10 min maximum in comparison with anatase systems (Table 2). The results presented confirmed it. The peak of phenol at 270-275 nm practically disappeared at a short contact time (Fig. 4).

Table 2 – The degradation rate of phenol (V , %/min) during UV action using samples

Sample	t , min	C , mg/l	V , %/min
anatase	10	39.0	2.20
	20	33.0	1.70
	30	23.0	1.35
P25	10	34.0	3.20
	20	26.0	2.40
	30	17.5	2.10
k1	10	33.0	3.40
	20	29.5	2.05
	30	24.0	1.73
m1	10	27.5	4.50
	20	12.5	3.75
	30	10.0	2.67

Note: C is the concentration of phenol after contact with the sample at different UV exposure times, taken from in Fig. 5

As for titanium dioxide, there may also be a potential barrier in the grain region. According to the authors, this is due to chemisorbed negative oxygen ions on the surface of TiO₂ grains. Electrons need to overcome the barrier in the grain region. The width and height of the barrier depend on the shape and size of the grain, number of boundaries, particle size, etc. Thus, doping TiO₂ with PANI allows strong electrostatic interaction with a decreasing potential barrier. The authors of [16-19] note that when PANI-TiO₂ composites are illuminated with UV light, both TiO₂ and PANI absorb photons to generate electron-hole pairs. The relative energy levels of PANI (HOMO, p -orbital and LUMO, π^* -orbital) and TiO₂ (conduction band, CB, and valence band, VB), create a synergistic effect. Photogenerated holes in the TiO₂ VB can directly transfer to the HOMO of PANI. Simultaneously, photogenerated electrons can transfer to the TiO₂ CB, which results in charge separation and stabilization, thus hindering

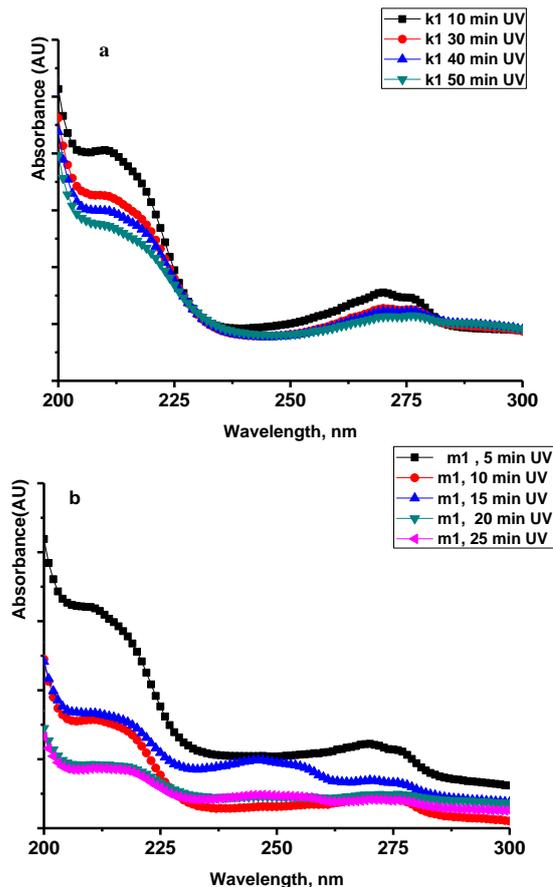


Fig. 4– UV-Vis spectra of phenol destruction using systems: k1 (a) and m1 (b)

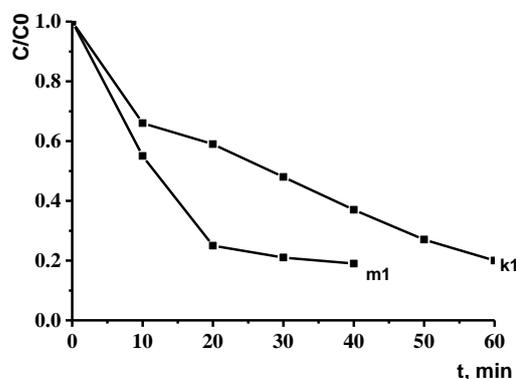


Fig. 5– Kinetics of photocatalytic degradation of phenol on the samples

the recombination process. As a result, electron-hole pairs are separated effectively, and the photocatalytic ability is improved remarkably. When PANI-TiO₂ composites are illuminated with visible light, PANI absorbs photons to induce $\pi-\pi^*$ transition, transferring excited-state electrons to the π^* -orbital. Based on the synergistic effect, excited-state electrons can be readily injected into TiO₂ CB. Simultaneously, a positively charged hole can be formed due to the migration of an electron from the TiO₂ VB to the π -orbital of PANI. Subsequently, excited-state electrons and holes can transfer to the surface to react with water and oxygen to yield hydroxyl and superoxide radicals, which will oxidize the or-

ganic pollutant (phenol). As a result, rapid charge separation and slow charge recombination occur, resulting in higher photocatalytic activity of TiO₂ composites.

A mathematical analysis of the results of Table 2 and Fig. 5 was performed. The data were processed by interpolation methods. Newton fourth and sixth order polynomials $Pn(t) = C/C_0$ ($n = 4, 6$) were used in the same way as in the study of the rheology of nanocomposite suspensions in [24, 25]. The curves were plotted at 5 and 7 points, lines 1 and 2 correspond to the cases of anatase and P25, lines 3, 4 – to the cases of k1 composite with anatase and m1 composite with P25 nanoparticles, respectively (Fig. 6).

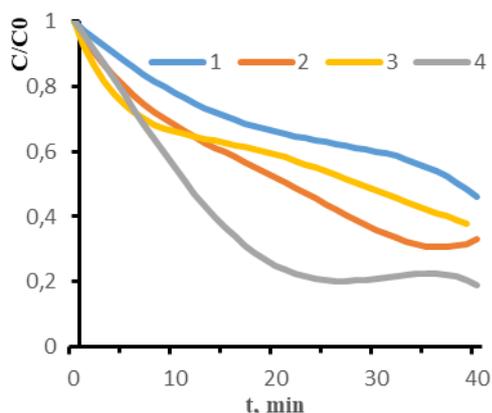


Fig. 6– Interpolation curves to samples: 1 – anatase, 2 – P25, 3 – k1, 4 – m1

The obtained results allow to draw the following conclusion. The combination of PANI nanoparticles with TiO₂ P25 will create an excited state of electron (e^-) and hole (h^+) pairs, which can react with O₂ and water vapor in the atmosphere to produce superoxide ions (O₂⁻) and hydroxyl radicals (OH•) under irradiation. Both O₂⁻ and OH• are extremely powerful agents in the destruction of toxic chemical compounds (dyes, phenol) to form CO₂ and water. This makes it possible to increase the performance of the photocatalyst and

the duration of its operation until the next regeneration. Due to its electronic structure and conductivity, PANI produces important h^+ .

4. CONCLUSIONS

In summary, a thin layer of PANI on the surface of TiO₂ particles has been successfully prepared via *in situ* polymerization method. The particles exhibited a photocatalytic effect on the degradation of phenol under UV and visible light irradiation compared with pure anatase TiO₂ nanoparticles and P25. PANI film is a good sensitizer after UV irradiation. The residual concentration of phenol decreases for composites P25 in comparison with other systems, so, faster degradation of phenol occurs at a short contact time. The excellent photocatalytic effect of PANI-TiO₂-P25 is attributed to the synergistic effect between PANI and TiO₂, which promotes the migration efficiency of photogenerated carriers at the PANI-TiO₂ interface (EPR). The experimental data were processed by interpolation and curves were constructed, illustrating the rate of degradation of pollution (phenol) concentration. This should be useful in subsequent analytical studies. It was stated that the degradation rate V (%/min) is maximum in the first 10 min. The proposed method can be used for the synthesis of TiO₂ nanocomposites with various conducting polymers. Overall, conducting polymer sensitized TiO₂ composites represent a promising method for addressing environmental pollution.

ACKNOWLEDGEMENTS

This research was funded by the National Academy of Sciences of Ukraine, grant No. 528/IPM-11/20.

The authors express gratitude to Tomila T.V., Lobunets T.F. (Institute for Problems of Materials Science, NAS of Ukraine), Prof. Lyubchik S. (Technical University NOVA, Lisbon), Prof. Christophe Colbeau-Justin, PhD Ghazzal M.N., PhD Teseer Bahry, Prof. H. Remita of Laboratory photocatalysis at University Paris Sud.

REFERENCES

- M. Zahorny, *Powder Metall. Met. Ceram.* **56**, 130 (2017).
- I. Papagiannis, G. Koutsikou, Z. Frontistis, I. Konstantinou, G. Avgouropoulos, D. Mantzavinos, P. Lianos, *Catalysts* **8**, 455 (2018).
- Y. Duan, L. Liang, K. Lv, Q. Li, M. Li, *Appl. Surf. Sci.* **456**, 817 (2018).
- M.N. Lyulyukin, P.A. Kolinko, D.S. Selishchev, D.V. Kozlov, *Appl. Catal. B: Environ.* **220**, 386 (2018).
- G.V. Sokolsky, M.N. Zahorny, T.F. Lobunets, N.I. Tyschenko, A.V. Shyrokov, A.V. Ragulya, S.V. Ivanov, N.V. Gayuk, V.E. Sokol'skii, L. V. Zudina, *J. Chem. Technol.* **27**, 130 (2019).
- J. Li, N. Wu, *Catal. Sci. Technol.* **4**, 4440 (2014).
- M. Zahorny, *Functional Nanocomposites Based of Titanium Dioxide* (Mauritius: LAP Lambert Academic Publishing: 2018).
- V. Gilja, K. Novaković, J. Travas-Sejdic, Z. Hrnjak-Murgić, M. Kraljić Roković, M. Žic, *Nanomaterials* **7**, 412 (2017).
- T.J. Brooms, B. Otieno, M.S. Onyango, A. Ochieng, *J. Environ. Sci. Health A* **53**, 99 (2017).
- H Xu, F. Jia, Z. Ai, L. Zhang, *Cryst. Growth Des.* **7**, 1216 (2007).
- M.N. Ghazzal, H. Kebaili, M. Joseph, D.P. Debecker, P. Eloy, J. De Coninck, E.M. Gaigneaux, *Appl. Catal. B: Environ.* **115-116**, 276 (2012).
- A.L. Luna, D. Dragoe, K. Wang, P. Beaunier, E. Kowalska, B. Ohtani, C. Colbeau-Justin, *J. Phys. Chem. C* **121**, 14302 (2017).
- I.F. Myronyuk, V.O. Kotsyubynsky, V.M. Boychuk, I.M. Mykytyn, V.M. Gun'ko, *J. Nano- Electron. Phys.* **13** No 1, 01001 (2021).
- M.V. Bondarenko, T.A. Khalyavka, A.M. Melnyk, S.V. Camyshan, Ya.V. Panasuk, *J. Nano- Electron. Phys.* **10** No 6, 06039 (2018).
- F. Wang, S.X. Min, *Chinese Chem. Let.* **18**, 1273 (2007).
- S. Ghosh, N.A. Kouamé, L. Ramos, S. Remita, A. Dazzi, A. Deniset-Besseau, H. Remita, *Nat. Mater.* **14**, 505 (2015).
- Y. Zhu, S. Xu, D. Yi, *Reac. Funct. Polym.* **70**, 282 (2010).
- K.S. Ajay, V. Rishi, K.J. Praveen, C. Umesh, K.J. Vipin, *J. Nano- Electron. Phys.* **11** No 2, 02012 (2019).
- A. Hashemi Monfared, M. Jamshidi, *Prog. Organ. Coat.* **136**, 105300 (2019).
- D.C. Hurum, A.G. Agrios, K.A. Gray, T.R.M.C. Thurnauer,

- J. Phys. Chem. B* **107**, 4545 (2003).
21. X. Xin, T. Xu, J. Yin, L. Wang, C. Wang, *Appl. Catal. B: Environ.* **176-177**, 354 (2015).
22. F. Karray, A. Kassiba, *Physica B* **407**, 2119 (2012).
23. A.L. Kon'kin, V.G. Shtyrin, R.R. Garipov, A.V. Aganov, A.V. Zakharov, V.I. Krinichnyi, P.N. Adams, A.P. Monkman, *Phys. Rev. B* **66**, 075203 (2002).
24. O.V. Kuzma, 2017 *IEEE 10th International Conference Nanomaterials: Applications & Properties (NAP)* **1**, 01PCSI32 (2017).
25. O.V. Kuzma, 2020 *IEEE 10th International Conference Nanomaterials: Applications & Properties (NAP)* **1**, 01NSSA13 (2020).

Оптична й фотокаталітична активність нанокompозитів ПАН/TiO₂ з наночастинками анатаза і P25

М.М. Загорний¹, Н.І. Тищенко¹, А.В. Рагуля¹, О.М. Лавриненко¹, А.М. Касумов¹,
А.К. Мельник², О.В. Кузьма³, А.І. Євтушенко¹

¹ Інститут проблем матеріалознавства НАНУ імені І.М. Францевича, вул. Кржижановського, 3, 03142 Київ, Україна

² Інститут сорбції та проблем ендоекології, вул. Генерала Наумова, 13, 03164 Київ, Україна

³ Національний технічний університет України «Київський політехнічний інститут імені Ігоря Сикорського», просп. Перемоги 37, 03056 Київ, Україна

У роботі поліанілін (ПАН) синтезований на поверхні наночастинок TiO₂ різної природи. Морфологію, розмір частинок, оптичну активність та фотокаталітичні характеристики отриманих матеріалів систематично вивчали різними аналітичними методами. Ультрафіолетова і видима, ЕПР спектроскопії нанокompозитів ПАН-TiO₂ підтвердили фізичну взаємодію між полімером та наночастинками TiO₂. Результати ЕПР показують, що нанокompозитний зразок m1, у якому ПАН зберігає більш упорядковану структуру, може покращити фотокаталітичну активність. Фотокаталітичні властивості нанокompозитів ПАН-TiO₂ досліджували шляхом деструкції фенолу (50 мг·л⁻¹) під УФ опроміненням. Результати показали, що деструкція фенолу відбувається максимально перші 10 хв для систем з P25 у порівнянні з системами анатазу. Встановлено, що максимальна швидкість деструкції V фенолу 4.2 %/хв характерна для зразку m1 (ПАН-TiO₂-P25). Показано, що поліанілінова плівка є сенсibiliзатором під час УФ опромінення. Фотокаталітичний ефект ПАН-TiO₂ пояснюється синергетичним ефектом між ПАН і TiO₂, що сприяє ефективності міграції фотогенерованих носіїв на міжфазній границі ПАН-TiO₂ (ЕПР). Математичний аналіз ілюструє швидкість деградації фенолу за рахунок кривих з поліномами 4 і 6 степенів.

Ключові слова: Фотокаталізатор, TiO₂, Анатаз, Поліанілін, Дірка, УФ-видимий, Нанокompозит, Опромінення.