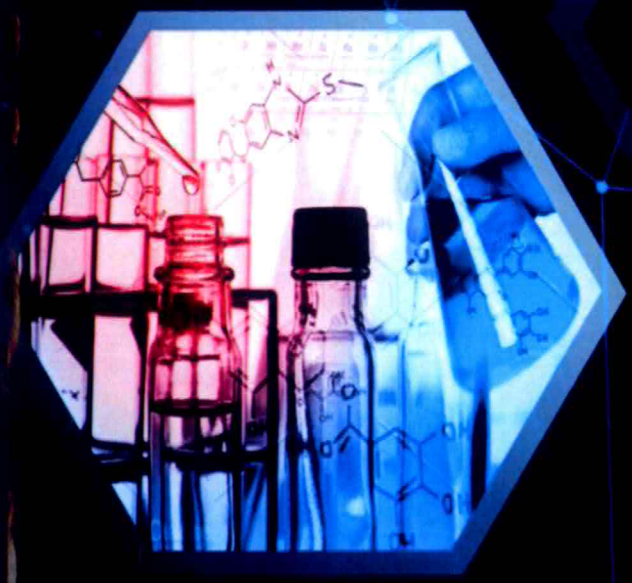
Proceedings of National Conference On

INNOVATIVE RESEARCH IN MEDICAL CHEMISTRY



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Dr.J.Jani Matilda

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DEPARTMENT OF CHEMISTRY

MUSLIM ARTS COLLEGE

THIRUVITHANCODE - 629167, KANYAKUAMRI DIST

TAMIL NADU - INDIA

Dept of Chemistry
Muslim Arts College

INNOVATIVE RESEARCH IN MEDICINAL CHEMISTRY

National Conference Proceedings

IRIMC-2023

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Dr. J. Jani Matilda

DEPARTMENT OF CHEMISTRY
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Preface.....

One Day National Conference On '**Innovative Research in Medicinal Chemistry**' **(IRIMC-2023)** organized by the Department of Chemistry, Muslim Arts College, Thiruvithancode on 10th February 2023. This seminar will be forum to specialize in the recent Innovation and to develop new therapeutic agents by involving synthetic organic and inorganic metal complexes in Medicinal Chemistry. We trust that this seminar would provide valuable insights to the participants to explore the deeper levels of chemistry towards the healthier life. We believe that the book of proceedings will be very useful and readable. It includes two invited talks and forty four contributed papers from research scholars, academicians and scientists. We thank all authors for their contributory papers. We look forward to a productive and successful seminar.

I take this opportunity to thank the Management, the Correspondent-Secretary and Principal of Muslim arts college, Thiruvithancode, for their unstinted cooperation, help and support. I must also thank all the conference office bearers, the organizers, members of the editorial board for their dedication, commitment and involvement in rendering the event unique and memorable. My thanks are also due to all the delegates and the scholar who really make a conference a conference with their paper presentation and sharing of notes, as it were, which is the very vital element in any intellectual activity for the benefit and betterment of humanity.

Dr. J. JANI MATILDA

About the conference

The Conference aims to provide a platform to the students, researchers and faculties of various nearby colleges and departments and also researchers from other institutes to come together and share their findings in various branches of chemistry. This conference will be one of the national meetings exclusively dedicated to medicinal chemistry. The national conference on innovative research in medicinal chemistry explores the deeper levels of chemistry towards a healthier life. The scientific session comprises research areas of Medicinal Chemistry, Bio Chemistry, Inorganic and Organic Materials, Coordination Chemistry, Polymer Chemistry, Nanoscience & Materials, Photo Chemistry, Environmental Chemistry etc. The very attractive speaker of the conference provides a unique opportunity to the participants to listen, interact and benefit from the invited talks and discussions.

MAGNETIC AND PHOTOLUMINESCENCE ANALYSIS OF PVP-TIO_2 AND CO, NI DOPED ZNO NANO PARTICLES AND THEIR ANTIMICROBIAL ACTIVITIES

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Abstract

The PVP encapsulated Titanium dioxide (TiO_2) nanoparticles optimize optical properties and magnetic behavior and also the Co and Ni doped ZnO nanoparticles was studied. The Nanosized metal oxide nanoparticles PVP-TiO_2 and Ni and Co –doped ZnO nanoparticles are being generated for ultimate use in medical practices that nanoparticles with smaller particle size were reported to show good antimicrobial and anti biofilm activity. These nanoparticles are smaller in size compared to bacterial pores that have a unique ability of crossing the cell membrane and killing the bacteria. In present work the $TiO_2$and Ni and Co doped nanoparticles were evaluated in their applicability in increasing antimicrobial and anti biofilm activities against Bacillus subtilis (B.Subtilis), Staphylococcus aureus (S.aureus), Salmonella typhi (S.typhi) and Pseudomonas aeruginosa (P.Aeruginosa), and antifungal activities against C.Albicans.VSM and PL analysis also used to characterized the optical properties and magnetic behavior of the PVP-$TiO_2$and Co, Ni doped ZnO nanoparticle.

Key Words: PVP-TiO_2, Ni and Co doped ZnO Nanoparticle, Agar Disc Diffussion, Antimicrobial, Antibiofilm optical, Photoluminesence, VSM.

1. Introduction

Titanium dioxide and zinc oxide Nanoparticles has been widely used as photo catalyst in many environmental and energy applications due to its efficient photoactivity, stability, lowcost and safety to the environment and humans. These Nanoparticles prepared by using hydrothermal process under different calcinations temperature. The optical properties and magnetic behavior of PVP-TiO_2, Co and Ni doped Zno Nanoparticles are characterized by VSM, PL Analysis.

1.4 Mechanism of antibacterial action:

TiO_2 and ZnO nanoparticles- Hydrothermal synthesis

When PVP-TiO_2 and (Ni and Co-doped) ZnO nanoparticles interact with light, the electrons (e^-) are raised to the conduction band, the holes (h^+) are created in the valence band. An electron reacts with oxygen to generate superoxide radical (O_2^-) and it reacts with H^+ ions to produce (HO_2^-) radical. The holes react with water or hydroxyl ion to produce hydroxyl radicals (OH^-). Release of H^+ ions with (HO_2^-) produces molecules of hydrogen peroxide (H_2O_2) and it damages the carbohydrates, nucleic acids, lipids, proteins, DNA and amino acids. The generation of ROS ($OH^- O_2^-$ And HO_2^-) has significant biological effects. Largely depends on the generation rate, rate of migration and energy levels of the excited electron-hole pair. The mechanism of light induced generation of ROS is given as,

$$PVP - TiO2/\ (Ni\ and\ Co)ZnO + h\gamma \rightarrow e^- + h^+$$

$$h^+ + H_2O \rightarrow OH^- + H^+$$

$$e^- + O_2 \rightarrow O_2^-$$

$$O_2^- + H^+ \rightarrow HO_2^-$$

$$HO_2^- + H^+ + e^- \rightarrow H_2O_2$$

2. Materials and Methods:

2.1. Preparation of PVP- TiO_2 Nanoparticle calcined at 500,600,700^{0}C.

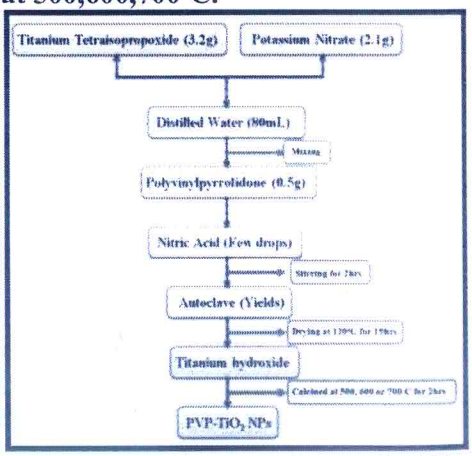

Figure.1 shows the Flow chart diagram of PVP-TiO_2 NPs

2.2 Preparation of PVP-TiO_2 NPs

Present work, 3.25g of cationic precursor (TTIP) and 2.12g of anionic precursor (KNO_3) was dissolved in 80mL of distilled water. In addition 0.5g of PVP was added. Then, a few drops of HNO3 were added to adjust the pH as

well as restrain the hydrolysis process under stirring for 2hrs. The above mixed solution was transferred into a 100mL Teflon-lined stainless autoclave and maintained at 180°C for 2hrs at a ramping rate of 5°/min. Then, obtained powder was obtained and calcined at 500°C for 3hrs. The similar procedure was followed for the preparation of PVP-TiO_2 calcined at 600°C and 700°C.

2.3 Preparation of (Ni and Co)-doped ZnO Nanoparticles:

In the present work, 3.45 g of zinc acetate and 2.5 g of NaOH were dissolved in 80 mL of distilled water under stirring for 2 hrs. The above mixed solution was transferred into a 100 mL of Teflon-lined stainless autoclave and maintained at 180 °C for 12 hrs. The precipitate was filtered and cleaned with acetone several times to remove impurities. Finally, the obtained samples were calcined at 450 °C for 2 hrs. The same procedure was followed for the preparation of ZnO: Ni^{2+} and ZnO:Co^{2+} NPs

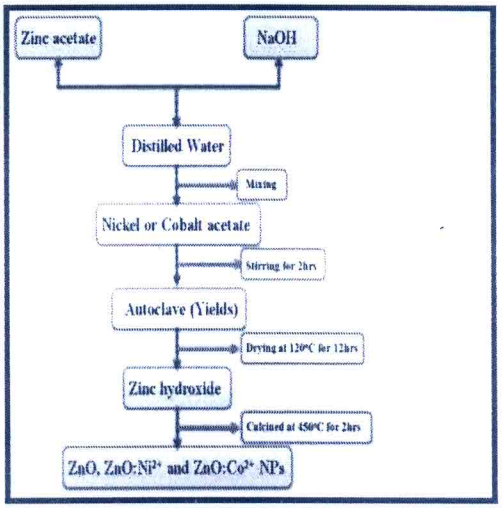

Fig1.1Shows the Flow chart diagram of as-prepared ZnO samples

3. Result and Discussion:

3.1 PL Analysis of PVP TiO_2

PL spectra of the TiO_2 NPs calcined at 500, 600 and 700°C as shown in Fig. The emission spectra were observed in UV region at 348nm with an excitation wavelength of 325 nm. The UV emission originated from an excitonic recombination can be attributed to the surface a defect corresponds to the near-band-edge emission of TiO_2 NPs. The high UV emission indicates a good crystal quality and low density of surface defects of the obtained products, that there is change in the broadening of the emission peaks by the increase of calcinations temperature, which indicates that the uniform particle size and increased surface defects and it is used for optoelectronic devices in nanoscale region.

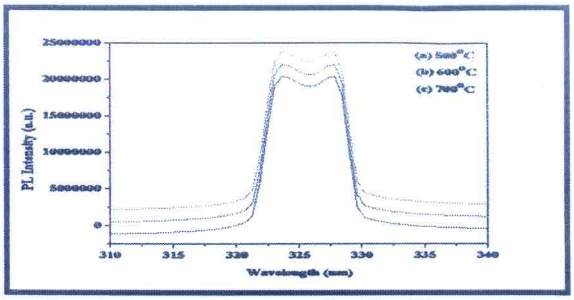

Fig1.3: Shows the PL of TiO_2 NPs at 500, 600 and 700°C

3.2 VSM Analysis of PVP-TiO_2

Magnetic behavior of the PVP-TiO_2 NPs calcined at 500°C as shown in Fig1.4. It is clearly seen that the magnetization values are increases rapidly at lower fields, which is indicates their ferromagnetic behavior. The saturated magnetizations (M_s) for the PVP-TiO_2 NPs are found to be 0.19emu/g and coercive forces (H_c) is 129Oe. Therefore, obtained ferromagnetism in the PVP-TiO_2 NPs was confined to the surface of the NPs, which is due to oxygen vacancies with strong magnetization at room temperature and it is used for spintronic devices applications.

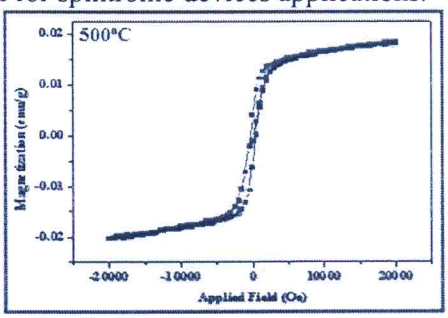

Fig1.4Shows the VSM of TiO_2 NPs at 500°C

3.3 PL Analysis of Co&Ni)Doped ZnO Nanoparticle:

Fig1.5. shows the emission spectra of the ZnO, ZnO:Ni^{2+} and ZnO:Co^{2+} NPs calcined at 450 °C. The characteristic peak of excitation wavelength was observed at 325 nm. Generally, ZnO shows three types of PL emissions. (i) PL spectra were observed in the UV emission at 380 nm and it can be attributes to free excitons recombination. (ii) PL spectra were observed in the blue (460 nm) and green (540 nm) emission, this was due to intrinsic defects including in Zn and O interstitials. (iii) PL spectra were observed in the green (630 nm) emission due to

recombination of delocalized electrons with holes in oxygen interstitials.

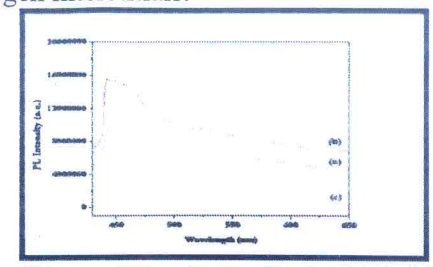

Fig.1.5 Shows PL of the ZnO, ZnO:Ni^{2+} and ZnO:Co^{2+} NPs calcined at 450 °C

The PL emission spectra of obtained products present two emission peaks in the UV and visible region. (i) UV region correspond to near band edge (365 nm) and (ii) visible region corresponds to trap sate emission (460 nm). From UV emission, it can be originate from recombination of free excitons through excitons-excitons collisions process responsible for photocatalytic degradation of dye. From visible emission, it can be attributed to recombination of photo generated holes with ionized charge states of intrinsic defects like in oxygen vacancies, interstitial and etc. The above result of PL spectra implies that the ZnO:Co^{2+} nanorods have been found to be favorable for optoelectronic devices and it is strongly affected by defects and impurities compared to ZnO and ZnO:Ni^{2+} NPs.

3.4 Antifungal Activity of pure and PVP-TiO_2 nanoparticles :

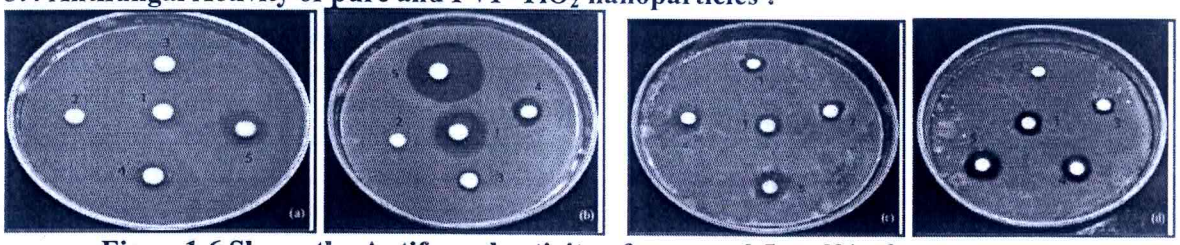

Figure1.6 Shows the Antifungal activity of pure and 5 mol% of PVP-TiO_2 Nanoparticle (a-b) *C. albicans*, (c-d) *A. Niger* fungal pathogens

The antifungal activity of pure and PVP-TiO_2 nanoparticles were performed against two fungal strains (*C. albicans, A. niger*) are shown in Figure 1.6(a-d), respectively. *C. albicans* (16 mm) shows maximum ZOI for PVP-TiO_2 nanoparticles compared to that of pure sample (12 mm), and minimum zone inhabitation for A. niger (10 mm) than that of the pure PVP-TiO_2 nanoparticles (6 mm) .

3.5 Antifungal activity of Ni and Co-doped ZnO nanoparticles

To study the antifungal property of Ni and Co-doped ZnO nanoparticles against the fungal pathogens (*C. albicans, A. Niger*) respectively. Antifungal activity of Ni and Co-doped ZnO nanoparticles against human pathogenic fungal is presented in Figure 1.7 (a-d). The variations in the ZOI with respect to Ni and Co-doped ZnO nanoparticles and it could be seen that the Co doped sample concentration of (100 µg/mL) is more prominent in cell inhibition against *C. albicans* (13 mm) and *A. niger* (12 mm) than that of Ni doped sample and also the inhibition of all the other tested bacteria is comparable to standard antibiotics Ketoconazole.

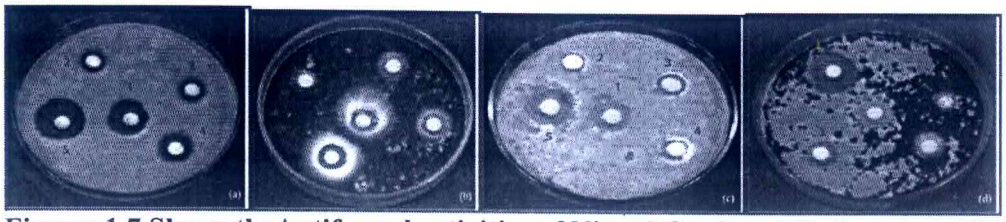

Figure: 1.7 Shows theAntifungal activities of Ni and Co-doped ZnO nanoparticles (a-b) *C. albicans*, (c-d) *A. Niger* fungal pathogens

3.6 Antibiofilm activity of PVP-TiO_2 and Co and Ni doped ZnO Nanoparticle.

Synthesized nanoparticles were tested for antibiofilm activity on four different bacteria and one fungus with different concentration ranging from 125µg/mL to 500µg/mL. All the concentration showed different ranges of antibiofilm activity depend on the concentration . In the present study, the PVP-TiO_2 nanoparticles show maximum concentrations of (500 µg/mL). The antibiofilm activities of PVP-TiO_2 were 89.09% for *B. subtilis*, 71.17% for *S. aureus*, 70.94% for *S. typhi*, 89.32% for *P. aeruginosa* and 90.15% for *C. albicans*. For Co-doped ZnO nanoparticles show maximum concentrations of 85.41% for *B. subtilis*, 73.67% for *S. aureus*, 86.83% for *S. typhi*, 88.14% for *P. aeruginosa* and 86.43% for *C albicans* .

4.Conclusion:

In this work presents the synthesis and magnetic behavior and optical properties of PVP-$TiO_2$and Co,Ni doped ZnO nanoparticles.PVP TiO_2,Co&Nidoped ZnO Nps prepared through a simple hydrothermal method under various calcinations temperature.These Nanoparticles showed significant zones of inhibition for antimicrobial activity,were performed by using the Agar Disc Diffusion method and Minimum inhibitory concentration method aginst four pathogens.The optical properties of of opyical bandgap are dependent on the calcinations temperature,this was due to lower calcinations temperature have high optical band gap energy than the other calcinations temperature and it is used for optical device applications.magnetic behavior of the PVP-TiO_2 ,Co&Ni doped ZnO nanoparticles,its clearly seen the that the magnetization values increases rapidly at lower fields,which is indicates their ferromagnetic behavior.Its used for spintronics device aaapplication.

5.References :

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DEPARTMENT OF CHEMISTRY

National Conference On

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Certificate

This is to certify that ~~Mr/Ms/Mrs~~/Dr. J. ARUL HENLY SHEELA, Asst. professor, Muslim Arts College Thiruvithancode has participated in the National Conference on Innovative Research in Medicinal Chemistry (IRIMC-2023) organized by the Department of Chemistry, Muslim Arts College, Thiruvithancode, Kanyakumari District on 10th February 2023.

He/She has presented a paper Oral/Poster entitled Magnetic And Photoluminescence Analysis Of PVP-TiO_2 And LO.N.I. DOPED ZNO Nano Particles And Their Antimicrobial Activities.

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Secretary

Dr. G. Edwin Sheela
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