

**UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002**

**UGC Major Research Project (SR)
FINAL PROJECT REPORT**

1. TITLE OF THE PROJECT

Investigation of photocatalytic response of TiO₂ nanostructures under doping and irradiation for practical applications.

2. NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATOR

Name: Dr. Gazi Ameen Ahmed

Address: Department of Physics, Tezpur University, Tezpur-784028, Assam, India.

3. NAME AND ADDRESS OF THE INSTITUTION

Tezpur University, Tezpur-784028, Assam, India.

4. UGC APPROVAL NO. AND DATE

F.No. 42-785 / 2013 dated 1st April 2013.

5. DATE OF IMPLEMENTATION

1st April, 2013

6. TENURE OF THE PROJECT

1st April 2013 to 31st March 2017

7. TOTAL GRANT ALLOCATED

Rs.13,97,800/-

8. TOTAL GRANT RECEIVED

Rs.13,00,000/-

9. FINAL EXPENDITURE

Rs.8,69,117/-


8.11.17

10. TITLE OF THE PROJECT

Investigation of photocatalytic response of TiO₂ nanostructures under doping and irradiation for practical applications.

11. OBJECTIVES OF THE PROJECT

The photocatalytic activity of TiO₂ is characterized by high reaction rates and short treatment times due to rapid oxidation reactions by hydroxyl radicals. Although the deep root of photocatalytic properties are directly related to its crystallite size and defect structures but in addition its structural properties including surface area, porosity, morphology, and pore size distribution are of great importance. In our work we were to try to explore nanotechnology and new material chemistry procedure for the synthesis of TiO₂ photo-catalysts with the desirable properties mentioned above. The work was originally planned to do the following tasks:

- Development of pure and doped Titanium Dioxide (TiO₂) nanostructures.
- Study of the Titanium Dioxide (TiO₂) nanostructures using different characterization tools viz. X-ray Diffraction, UV-Vis spectroscopy, Electron microscopy etc.
- Study of the modification of the doped and undoped Titanium Dioxide (TiO₂) nanostructures through various process specially ion irradiation.
- Analysis of the Photoluminescence response and Raman spectra for the study of the optical properties of the nanostructure systems.
- Variation of electrical transport properties of the virgin and modified nanostructures will be studied under different illumination conditions and for different wavelengths.
- Finally, to study its applicability in photocatalytic applications.

12. WHETHER OBJECTIVES WERE ACHIEVED

- Mn²⁺ doped TiO₂ nanoparticles were synthesized
- XRD, UV-Vis spectroscopy and TEM analysis was performed.
- Raman spectra studies and photo-luminescence studies were performed.
- Photocatalytic activity of these materials were studied.

13. ACHIEVEMENTS FROM THE PROJECT

The optical, magnetic and photocatalytic properties of doped and undoped TiO₂ noncrystalline matter were found through the work carried out in this project.

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8-11-17

14. SUMMARY OF THE FINDINGS

(IN 500 WORDS)

The influence of Gadolinium doping on structural, optical and photocatalytic properties of TiO₂ nanoparticles was studied. The doped photocatalysts are found to exhibit enhanced photocatalytic activity compared to undoped TiO₂. The abinitio calculation based on density functional theory shows that the Gd ions are localized, indicating that they mainly act as charge carrier trapping centers and delay the electron-hole recombination rate beneficial for enhanced photocatalytic activity.

Fig.1 shows the XRD pattern of Gd doped TiO₂ samples. All the peaks in the samples are well indexed to the tetragonal anatase phase (JCPDS-782486) and no hint of Gadolinium containing oxide phases are resolved. The average crystallite size are calculated by using the Scherrer's formula $d = 0.9\lambda / \beta \cos\theta$ where λ = wavelength of the X-ray source used; β = full width at half maximum (FWHM); θ = Bragg diffraction angle. The average crystallite size for pristine TiO₂ (0.00 mol) is calculated to be 7.8 nm and 5.9 nm, 5.45 nm, 5.42 nm for 0.03, 0.05 and 0.07 mol of Gd respectively. The decrease in the size after doping is attributed to the repulsive interactions between dopant ions that prevents coalescence of the nanocrystallites and inhibits the growth by formation of Gd-O-Ti bond. The width of the diffraction peak increases with the increase in doping concentration indicating systematic decrease in grain size and degradation of the structural quality after doping.

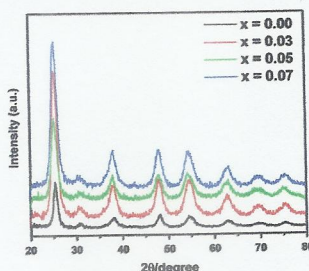


Fig. 1. X-ray diffraction pattern of (a) undoped and (b) Gd doped TiO₂ nanoparticles.

The role played by non-magnetic Mn on the magnetic properties of TiO₂ nanoparticles was also studied. The samples display complete paramagnetic behavior at room temperature as well as at 10 K. Paramagnetism might be associated with the presence of isolated magnetic spins of Mn²⁺ in the system. Observation of negative Curie-Weiss temperature indicates presence of anti-ferromagnetic interaction in the system. Direct exchange interaction of Mn²⁺-Mn²⁺ and anti ferromagnetic super exchange interaction of Mn²⁺ ions via lattice O₂-ions contribute to anti ferromagnetism. Surprisingly, ferromagnetism appears in pure and Mn doped (0.07 mol) TiO₂ nanoparticles on vacuum calcination. Although Mn doped TiO₂ displays ferromagnetism, there is a loss in magnetization as compared to the undoped TiO₂. It is speculated that low growth temperature during vacuum calcinations might have resulted in amorphous MnO phase separation. This could result in competing ferromagnetic-antiferromagnetic interactions and overall reduction in magnetization. From the results it is evident that TiO₂ could be made ferromagnetic by introducing sufficient concentration of oxygen vacancies in the system. Mn doping, however, has an adverse effect on the overall ferromagnetic ordering, as there is possibility of antiferromagnetic d-d exchange interaction of Mn²⁺ ions as well as possibility of antiferromagnetic manganese oxide phases separation.

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15. CONTRIBUTION TO THE SOCIETY

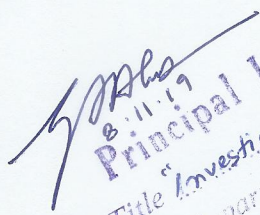
Knowledge of the synthesized nanoparticles may help in creating beneficial products.

16. WHETHER ANY PH.D. ENROLLED/PRODUCED OUT OF THE PROJECT

One (Dr.Susmita Paul).

17. NO. OF PUBLICATIONS OUT OF THE PROJECT Five

1. Susmita Paul, Biswajit Choudhury and Amarjyoti Choudhury, Magnetic property study of Gd doped TiO₂ nanoparticles, *Journal of Alloys and Compounds* 601 (2014) 201–206.
2. Susmita Paul and Amarjyoti Choudhury, Investigation of the optical property and photocatalytic activity of mixed phase nanocrystalline titania, *Appl. Nanosci.* 4 (2014) 839-847.
3. Susmita Paul, Amarjyoti Choudhury and Gazi Ameen Ahmed, Effect of Oxygen Vacancy on the room temperature magnetic behaviour of manganese doped nanocrystalline titania, *PIJMS* 1 (2014) 17-22.
4. Biswajit Choudhury, Susmita Paul, Gazi Ameen Ahmed and Amarjyoti Choudhury, Adverse effect of Mn doping on the magnetic ordering in Mn doped TiO₂ nanoparticles, *Mater. Res. Express* 2 (2015) 1-11.
5. Susmita Paul, Pawan Chetri, Biswajit Choudhury, Gazi Ameen Ahmed and Amarjyoti Choudhury, Enhanced visible light photocatalytic activity of Gadolinium doped nanocrystalline titania: An experimental and theoretical study, *Journal of Colloid and Interface Science* 439 (2015) 54-61.


Principal Investigator
Title "Investigation on applications"
Department of Physics
TEZPUR UNIVERSITY

(PRINCIPAL INVESTIGATOR)



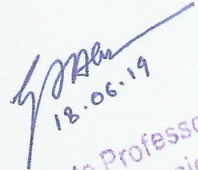
(REGISTRAR/PRINCIPAL)

Registrar
Tezpur University
Napaam, Tezpur

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI-110002

Final Consolidated item wise Audited Statement of Expenditure of major research project under the scheme for support of research as UGC Major research project:

1. Name of the Principal Investigator: Dr Gazi Ameen Ahmed
2. Dept. of University/College: Dept. of Physics, Tezpur University
3. U. G. C. approval No. & Date: F.42-785/2013 (SR) dated April 01, 2013
4. Title of the research project: "Investigation of photocatalytic response of TiO₂ nanostructures under doping and irradiation for practical applications"
5. (a) Effective date of starting the project: June 06, 2013
(b) Date of closing of project: March 31, 2017
6. (a) Period of Expenditure: From April 01, 2013 to June 17, 2019


18.06.19
Associate Professor
Deptt. Of Physics
Tezpur University

(b) Details of Expenditure:

Sl. No.	Item	Amount Approved (in Rs.)	Amount Received (in Rs.) From April 01, 2013 to March 31, 2014	Expenditure Incurred (in Rs.) From April 01, 2013 to March 31, 2014	Amount Received (in Rs.) From April 01, 2014 to March 31, 2015	Expenditure Incurred (in Rs.) From April 01, 2014 to March 31, 2015	Amount Received (in Rs.) From April 01, 2015 to March 31, 2016	Expenditure Incurred (in Rs.) From April 01, 2015 to March 31, 2016	Amount Received (in Rs.) From April 01, 2016 to March 31, 2017	Expenditure Incurred (in Rs.) From April 01, 2016 to March 31, 2017	Total Expenditure Incurred (in Rs.) Entire period: 01/04/2013 to 31/03/2017	Total Balance (in Rs.) Entire period: 01/04/2013 to 31/03/2017	Interest by Bank from 01/04/2013 to 17/06/2019
1.	Books / Journal	60,000	60,000	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	60,000/-	46,158/-
2.	Equipment	4,00,000/-	4,00,000/-	52,667/-	Nil	3,21,601/-	Nil	Nil	Nil	Nil	3,74,268/-	25,732/-	
3.	Contingency	1,20,000/-	60,000/-	32,066/-	Nil	24,415/-	Nil	Nil	48,000/-	Nil	56,481/-	51,519/-	
4.	Field Work /Travel	60,000/-	30,000/-	18,103/-	Nil	26,980/-	Nil	Nil	24,000/-	Nil	45,083/-	8,917/-	
5.	Hiring Service	30,000/-	15,000/-	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	15,000/-	
6.	Chemicals/ Glassware	1,20,000/-	60,000/-	Nil	Nil	52,152/-	Nil	Nil	48,000/-	Nil	52,152/-	55,848/-	
7.	Overhead Charges (10% of approved recurring Grant except Travel & Field work)	79,800/-	79,800/-	59,850/-	Nil	Nil	Nil	19,950/-	Nil	Nil	79,800/-	Nil	
8.	Any other items (please specify)	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	
9.	Honorarium to Principal Investigator	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	Nil	

(c) Staff (Date of Appointment: 06-06-2013):

Sl. No.	Item	Amount Approved (in Rs.)	Amount Received (in Rs.) From April 01, 2013 to March 31, 2014	Expenditure Incurred (in Rs.) From April 01, 2013 to March 31, 2014	Amount Received (in Rs.) From April 01, 2014 to March 31, 2015	Expenditure Incurred (in Rs.) From April 01, 2014 to March 31, 2015	Amount Received (in Rs.) From April 01, 2015 to March 31, 2016	Expenditure Incurred (in Rs.) From April 01, 2015 to March 31, 2016	Amount Received (in Rs.) From April 01, 2016 to March 31, 2017	Expenditure Incurred (in Rs.) From April 01, 2016 to March 31, 2017	Total Expenditure Incurred (in Rs.) Entire period: 01/04/2013 to 31/03/2017	Total Balance (in Rs.) Entire period: 01/04/2013 to 31/03/2017
10.	Project Fellow at 14000/- p.m.	5,28,000/-	2,64,000	1,37,667/-	Nil	1,12,000/-	Nil	11,666/-	2,11,200/-	Nil	2,61,333/-	2,13,867/-

TOTAL		Amount Approved (in Rs.)	Amount Received (in Rs.) From April 01, 2013 to March 31, 2014	Expenditure Incurred (in Rs.) From April 01, 2013 to March 31, 2014	Amount Received (in Rs.) From April 01, 2014 to March 31, 2015	Expenditure Incurred (in Rs.) From April 01, 2014 to March 31, 2015	Amount Received (in Rs.) From April 01, 2015 to March 31, 2016	Expenditure Incurred (in Rs.) From April 01, 2015 to March 31, 2016	Amount Received (in Rs.) From April 01, 2016 to March 31, 2017	Expenditure Incurred (in Rs.) From April 01, 2016 to March 31, 2017	Total Expenditure Incurred (in Rs.) Entire period: 01/04/2013 to 31/03/2017	Total Balance (in Rs.) Entire period: 01/04/2013 to 31/03/2017	Interest by Bank from 01/04/2013 to 17/06/2019
		13,97,800/-	9,68,800/-	3,00,353/-	Nil	5,37,148/-	Nil	31,616/-	3,31,200/-	Nil	8,69,117/-	4,30,883/-	46,158/-

Balance as on 31/03/2017 : Rs. 4,30,883/-

Balance with Bank Interest as on 17/06/2019 : Rs. 4,77,041/-

2576119

[Signature]
18.06.19
Associate Professor
Dept. Of Physics
Tezpur University

- I. It is certified that the appointment has been made in accordance with the terms and conditions laid down by the commission
- II. If As a result of check or audit objective, some irregularity is noticed, at a later date, action will be taken to refund adjust or regularized the objected amounts.
- III. Payment @ revised rates shall be made with arrear on the availability of additional funds.

18.06.19
(Dr. Gazi Aman Ali)
Principal Investigator
Title "Investigation on applications"
D. partment of Physics
TEZPUR UNIVERSITY

Signature of
Principal Investigator
Associate Professor
Deptt. Of Physics
Tezpur University

[Signature]
Signature of
Finance Officer
Tezpur University
~~Finance Officer~~
Tezpur University
25/6/19

[Signature]
Signature of
Register
Tezpur University
(Seal)
Registrar
Tezpur University

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI-110002

FINAL UTILISATION CERTIFICATE

Certified that from the grant of, **Rs. 9.68,800/-** received from the University Grants Commission in the financial year **2013-2014** vide University Grants Commission letter No. **F.42-7855/2013 (SR)** dated **April 01, 2013** and **Rs. 3.31,200/-** received from the University Grants Commission in the financial year **2016-2017** vide University Grants Commission letter No. **F.42-7855/2013 (SR)** dated **July 12, 2016**, under the scheme for UGC Major research project entitled "**Investigation of photocatalytic response of TiO₂ nanostructures under doping and irradiation for practical applications**" and Bank Interest earned till **June 17, 2019** of **Rs.46,158/-** an amount of **Rs. 8.69,117/-** has been fully utilized in the entire project period **2013-2017** for the purpose for which it was sanctioned and the remaining balance of **Rs. 4,77,041/-** which includes **Bank Interest till June 17, 2019** will be returned as the project has ended on **March 31, 2017** in accordance with the terms and conditions laid down by the University Grants Commission vide NEFT UTR No. SBIN219238618059 dated 26-08-2019

YPRhs
18.06.19
(Dr. Gazi Ameen Ahmed)
Principal Investigator
Title "Investigation of photocatalytic response of TiO₂ nanostructures"
Department of Physics
TEZPUR UNIVERSITY

Signature of
Principal Investigator

Associate Professor
Deptt. Of Physics
Tezpur University

[Signature]
Signature of
Finance Officer
Tezpur University
Finance Officer
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Signature of
Registrar
Tezpur University
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