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**APPLICATION FOR ADMISSION TO Ph.D. PROGRAMMES**

Date of Application:27-06-2020

Department	CHEMISTRY	Application No.	20200150
Area of Research	NANO MATERIALS AND COMPUTATIONAL CHEMISTRY	Research Mode	FULL TIME

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Qualification						
Degree	Discipline	College/university	Year Passed	AVG/CGPA	Class	Mode
BSC	CHEMISTRY	ARUL ANANDAR COLLEGE	2013	58	SECOND CLASS	REGULAR
MSC	CHEMISTRY	ARUL ANANDAR COLLEGE	2020	68	FIRST CLASS	REGULAR

Experience				
Organization	Designation	Experience From	Experience TO	Work Nature
ARUL ANANDAR COLLEGE		1970-01-01	1970-01-01	

Payment Details				
Transaction ID	Reference	Date of transaction	Amount	Status
20200150_200630125929	SSBI8946943474	30-06-2020	600	SUCCESS

# **Design and development of high performance photocatalysts using theoretical and experimental methods**

Sonai Jeyaraj

## **Abstract**

Recently, we have synthesized  $\text{Sn}_3\text{O}_4$  based photocatalyst by hydrothermal method and measured its photocatalytic activity in my M.Sc project. In this proposal, I propose to investigate photocatalytic activity of Sn based materials for photocatalytic activity by using ab initio density functional theory (DFT) and time-dependent density functional theory (TDFT). In the recent past,  $\text{Sn}_3\text{O}_4$  has been shown to be a potential candidate for photoinitiated process in  $\text{H}_2$  reduction reactions. The  $\text{Sn}_3\text{O}_4$  has large band gap which can be tuned by doping. Several different  $\text{Sn}_3\text{O}_4$  based complexes can be designed using density functional theory with different geometries, electronic structures, and optical characteristics. Experimentally, it is highly time consuming and need a lots of resources to test the photocatalytic activities of all possible  $\text{Sn}_3\text{O}_4$  based complexes. In this situation, theoretical techniques such as DFT can easily guide experimental studies by screening materials and provide insights into the photoactivity of the complexes. The main aim of this proposal is to design and develop  $\text{Sn}_3\text{O}_4$  complexes for hydrogen production applications and to provide a direction for chemical synthesis of these photocatalysts. After finding the potential materials for photocatalysts, with the supervisor's advice, I will do experimental synthesis and measure the catalytic activities.

## **Introduction**

The need for the energy will never end and it is essential in the modern world. Hydrogen plays an important role in the energy sector. It is used in various industries including various chemical syntheses, fossil fuel separation, ammonia synthesis, onboard applications as fuel, etc. One of the most important and environmental friendly applications is water splitting using the phenomena of photocatalysis.

Currently other photocatalysts based on metal oxides, metal sulfides and metal nitrides are also gaining attention for water splitting applications in large amounts. These heterogeneous catalysts are semiconductors and their band gap leads to better photocatalytic activities compared to metals (zero band gap) and insulators (high band gap). In heterogeneous photocatalysis the same process occurs on the surface of the heterogeneous photocatalysis. So we need a suitable band gap for the design a photocatalyst with good photocatalytic activity. One of the ways is to tune the band gap of potential materials so that we can tune their photocatalytic activities. In photocatalytic reactions, trapping and recombination center between photogenerated electrons and holes results in a decreased photocatalytic activity in active sites. Some of the co-catalysis Pt, NiO and  $\text{RuO}_2$  are also used. These are unnecessary for oxide based photocatalysts.

For the past few decades,  $\text{TiO}_2$  photocatalysts are widely studied. Honda and Fujishima synthesised  $\text{TiO}_2$  photocatalysts for the first time early 1970s. When  $\text{TiO}_2$  is irradiated with UV light, the electron and hole pairs are generated which are relevant in the production of hydrogen. However the efficient splitting of water into  $\text{H}_2$  and  $\text{O}_2$  under visible light irradiation is not observed. Frank and Bard examined the possibility of using

TiO<sub>2</sub> to decompose cyanide in water which is of great interest for environmental applications. Now, TiO<sub>2</sub> is one of the most important ecofriendly photocatalyst because of its availability, economical and high stability.

Photocatalysts like TiO<sub>2</sub> has different forms Anatase and Rutile. Compared to Rutile for anatase has a high band gap. The crystallinity is increased by calcination. Some sacrificial agents also used to evaluate photocatalytic activity such as alcohol and a sulfide ions. It enhance the electrons in a photocatalyst.

Photocatalytic production of hydrogen has been paying attention to solve the energy and environmental problems. Generally, the photocatalyzed hydrogen production inherently proceeds via two charge processes, such as (a) the trapping of photo-generated electrons and holes on surface active sites of semiconductors, and (b) the interfacial transfer of electrons and holes from active sites to reacting substrates. In recent times, the metal/semiconductor and semiconductor/semiconductor composite materials are used to modify band gap position, improve carrier separation and facilitate charge recombination for photocatalytic generation of hydrogen. For this reason, construction of photocatalysts with some metal sulfides, metal oxides, and noble metals were useful to enhance the hydrogen generation.

Moreover, it has been reported that the structure and morphology of the photoactive sites of semiconductor to improve the light harvesting and photocatalytic activity. However, the efficiency, expensive and toxic nature of materials would also be calculated for practical applications. Very recently, non-toxic tin oxide (Sn<sub>3</sub>O<sub>4</sub>) sheet like structure photocatalysts have been shown to enhance the activity for hydrogen evolution. There is a lot of scope in the area in developing and enhancing Sn based photocatalysts. In this research, we propose design and develop Sn<sub>3</sub>O<sub>4</sub> based complexes for photocatalytic applications. We plan to use density functional methods to get useful insights in to the structural, electronic and photocatalytic activities followed by experimental synthesis and measurements.

### **What I have done so far**

In my present M.Sc project, with the guidance of my supervisor, I have synthesized a visible light driven Sn<sub>3</sub>O<sub>4</sub> supported bimetallic nanoparticles and have measured its photocatalytic activity using basic experimental techniques. I have been writing a paper and it is to be submitted soon. In the project titled “Facile Synthesis of Visible Light Driven Tin Oxide (Sn<sub>3</sub>O<sub>4</sub>) Supported Bimetallic Nanoparticles and its Photocatalytic Activity”, we have prepared Sn<sub>3</sub>O<sub>4</sub> based photocatalyst through two-step hydrothermal process and the photocatalytic activity has been examined by the generation of hydrogen. The synthesized Sn<sub>3</sub>O<sub>4</sub> supported photocatalyst has been characterized by XRD, TEM, EDX and XPS.

### **Objectives of this Proposal**

- To design Sn<sub>3</sub>O<sub>4</sub> based photocatalyst with various compositions
- To calculate the structural properties of Sn<sub>3</sub>O<sub>4</sub> with different compositions using DFT

- To calculate the electronic properties of Sn<sub>3</sub>O<sub>4</sub> using DFT
- To calculate the photocatalytic activities of Sn<sub>3</sub>O<sub>4</sub> with various compositions using DFT and time-dependent DFT.
- To design a novel Sn<sub>3</sub>O<sub>4</sub> based photocatalyst in effective manner other than hydrothermal method (for reducing the cost).
- To develop Sn<sub>3</sub>O<sub>4</sub> based semiconductors from changing several electronic characteristics like atomic configuration, bandgap energy, band position, and lifetime of electrons and holes using DFT followed by synthesis and experiments
- Doping with metals and nonmetals to enhance the visible-light response of Sn<sub>3</sub>O<sub>4</sub> photocatalysis (Au and Pd are currently used).
- To develop a Z-Scheme photocatalyst materials for production of hydrogen, environmental pollution and dye degradation.

## **Methodology**

This project has two parts.

### **1) Theoretical calculations:**

The theoretical calculations will be performed with the Kohn-Sham Density functional theory for the structural and electronic properties calculations of Sn<sub>3</sub>O<sub>4</sub> based photocatalysts. The photocatalytic activities will be studied by time-dependent density functional theory. At present I have been using ASE computational package (site) to study the catalytic activity of different substrates. I will start with this ASE package which is an open source code. Then, the calculations may be performed using Quantum Espresso code and other open source codes. At present, I have been using my laptop (4 GB RAM) to compute my calculations. Based on the availability of the resources at the university, I will use it. With the support of my Professor, I will collaborate with other research institutions where computation facility is available to complete my calculations.

### **2) Experimental Methods:**

After finding the potential Sn<sub>3</sub>O<sub>4</sub> based photocatalysts, with the help of the supervisor, I will synthesis selective photocatalysts and study their properties by various methods. Since in my MSc project, since I have synthesized a visible light driven Sn<sub>3</sub>O<sub>4</sub> supported bimetallic nanoparticles and have measured its photocatalytic activity using basic experimental techniques, I can start with the same procedure. The newly synthesized photocatalysts will be characterized by various techniques such as XRD, TEM, EDX and XPS.

## Research Outcome

- A complete understanding of Sn<sub>3</sub>O<sub>4</sub> based photocatalysts by using DFT/TDFT
- A 3-6 papers in peer-reviewed international journals from the results obtained using DFT/TDFT calculations and experimental studies.
- There is a possibility to enhance the band gap of the photocatalyst with computational methods using some open source software like python.
- Currently we are using this Sn<sub>3</sub>O<sub>4</sub> based photocatalyst is used for the production of hydrogen. In further research there is a possibility of some relevant photocatalytic applications such as removal of inorganic pollutants, water splitting, and organic synthesis.

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அறிவியற் புலம்  
FACULTY OF SCIENCE

மதுரை காமராசர் பல்கலைக்கழக ஆட்சிப்பேரவை

ஜெயராஜ். கோ. இப்பல்கலைக்கழகத்தில் இணைந்த

தன்னாட்சிக் கல்லூரியான அருள் ஆனந்தர் கல்லூரி, கருமாதூர்

விதித்திருந்த பாடப் பயிற்சியினையும் தேர்வினையும் நன்கு முடித்த பின்னர் ஏப்ரல் 2013 இல் நடைபெற்ற தேர்வில்

இரண்டாம் வகுப்பு பெற்று தேர்வுற்றார் எனக் கல்லூரித் தேர்வு ஏற்புக்குழு பரிந்துரைத்தவாறு.

வேதியியல் சிபிவில் அறிவியல் இளையர் பட்டம்

பெறுதற்கு உரியவர் ஆகின்றார் என இதன்வழி அறிவிக்கின்றது.

பல்கலைக்கழக இலச்சினையுடன் இது வழங்கப்படுகின்றது.

The Senate of the MADURAI KAMARAJ UNIVERSITY  
hereby makes known that J.EYARAJ S has been admitted to the

DEGREE OF BACHELOR OF SCIENCE IN CHEMISTRY

he/she having successfully completed the course of studies and examination prescribed therefor by the  
ARUL ANANDAR COLLEGE, KARUMATHUR

(an Autonomous College of this University) and upon the recommendation by the College Awards Committee and  
having been placed by them in the SECOND CLASS

at the Examination held in APRIL 2013

Register No. : 10CH1512

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பல்கலைநகர், மதுரை - 625 021  
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நாள் Dated 23 October 2013

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வேதியியல் சிபிவில் அறிவியல் இளையர் பட்டம்

பெறுதற்கு உரியவர் ஆகின்றார் என இதன்வழி அறிவிக்கின்றது.

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having been placed by them in the SECOND CLASS

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नाम / Name  
**JEYARAJ**

पिता का नाम / Father's Name  
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जन्म की तारीख / Date of Birth  
**21/05/1993**

*S. Jayaraj*

हस्ताक्षर / Signature



07012018



# India Driving Licence(Tamilnadu)

Form 7

DOI 28/04/2016

D.L.No : TN58 20160003051

Name : JEYARAJ S

S/D/W of : SONAI

Address

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UTHAPPANAYAKKANUR USILAMPATTI  
MADURAI

Temp Add:

SRI KARTHICK DRIVING SCHOOL

D.O.B : 21/05/1993 B.G.



Punishments

Licensed to drive throughout India, vehicles of the following descriptions  
M/CVCL WG 28/04/2016 TN58 LMV 28/04/2016 TN58

Non-Transport Veh. Valid upto 27/04/2036



*S Jeyaraj*

Signature/L.T.I  
of the Holder

*S. Jeyaraj*  
28/04/16

