PROPOSAL FOR THE ΣΠΣ UNDERGRADUATE RESEARCH AWARD

TITLE OF RESEARCH PROJECT: Design and Development of Novel Nanocomposite Materials and Reactor Systems for Photocatalysis

DURATION OF THE PROJECT: One Calendar Year

SPS CHAPTER OF TUSKEGEE UNIVERSITY, DEPARTMENT OF PHYSICS

ZONE: 06, SPS Chapter #7446

PROPOSAL SUBMITTED BY:

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SPS TU Chapter Faculty Advisor:	**Dr. Akshaya Kumar**	Akshaya Kumar

Amount Requested for implementing the research project: **$2000.00**

Date of Submission: **October 16, 2012**

EXECUTIVE SUMMARY

Photocatalysis is an interdisciplinary field of research which involves the contribution not only from Physicists, chemists, material scientists, chemical and environmental engineers, but also demands often the need of technologists who can build the custom made reactor systems for different applications. Novel solid state materials' development is equally important for the water/air decontamination and/or fuel generation processes. In this research study, we proposed to develop and demonstrate both aspects of reactor and materials' design for the sunlight assisted photocatalysis.

Materials' Development: Semiconductor oxide nanoparticles based on titanium oxide (TiO_2) has shown potential photocatalytic activity for destruction of toxic chemical contaminants in water/air by ultraviolet (UV) light irradiation. However, TiO_2 shows rather poor activity on these processes with exposure of only visible (sun) light. It is estimated that only 4% of the sunlight contains UV component and the large proportions (~96%) are with visible light wavelengths (>400 nm). While investigating the plain TiO_2, we understand that the poor catalytic activity under incandescent light was due to its high band gap (~3.2 eV) which needs further optimization procedures. Based on our extensive literature search, we found that Indium Vanadium Oxide ($InVO_4$) has not only low band gap values (1.8-2.0 eV), but also possess suitable band position in relation to the TiO_2 band edges. Therefore, in this research investigation, we proposed to develop novel TiO_2-Xwt.%$InVO_4$ nanocomposites that can utilize both UV and visible components of sunlight for both processes such as photo-oxidation to decontaminate water and photo-reduction to generate hydrocarbon.

Reactor Development: There is no companies manufacture the photocatalytic reactors for different applications. Moreover, the photocatalytic reactors' fabrication often relies on various experimental parameters including the amount of the photocatalysts and degradant, UV light intensity, air flow etc. Another aspect of the reactor design is based on the types such as continuous flow or batch processes. In this research study, we have proposed to develop custom build reactor system design which is suitable for specific photocatalytic applications. We will optimize the experimental parameters for obtaining the maximum efficiency and throughput. The materials' designed in the first part of the proposed study will be incorporated in this second part.

BACKGROUND

Purification of water from organic contaminants, disinfection of water and air [1-4], destruction of bacterial activity [5], non-polluting power generation (including solar energy) [6,7], reduction or stabilization of CO_2 [8, 9] and photodegradation of deep horizon oil spill [10] are the vital areas for urban, economic, environmental and industrial developments in the United States. Success in all of these areas strongly depends on the development and deployment of efficient, inexpensive, environmentally friendly and chemically stable catalysts and photocatalysts. Titanium dioxide (TiO_2) is widely used in many photocatalytic [11, 12] and water splitting [13, 14] applications because of its high stability, low cost, non toxic, high oxidation potential and chemically favorable properties. However, it can only utilize the ultraviolet portion of the solar spectrum, which results in low total efficiency of such catalyst in the sunlight energy utilization.

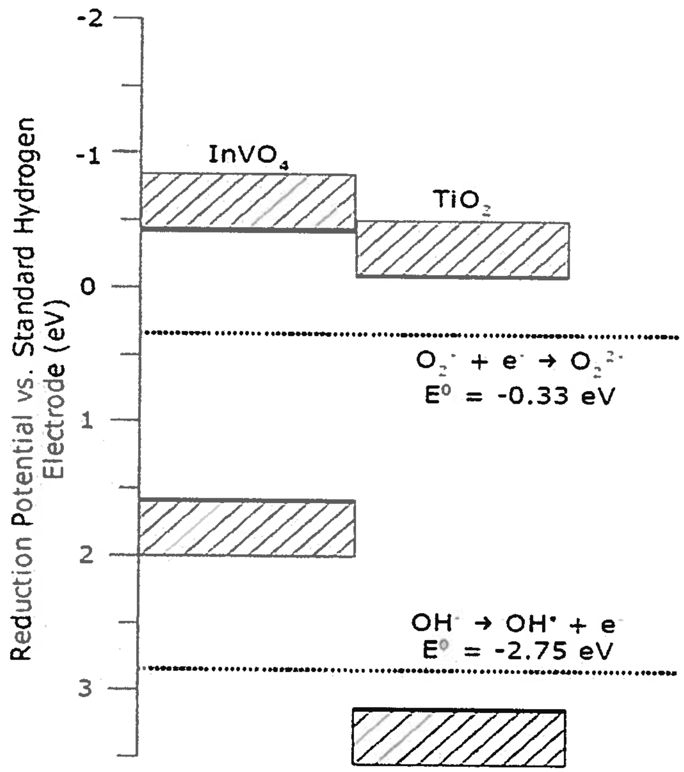

Figure 1: Band edge diagram of TiO_2 and $InVO_4$

Any improvements in photocatalytic efficiency of TiO_2 or development of other novel and new generation photocatalysts towards shifting their activity to the visible portion of the solar spectrum will have a significant impact. Indium vanadium oxide or Indium vanadate ($InVO_4$) is chosen as a viable photocatalyst with low band gap of 1.8-2.0 eV, and is demonstrated to split water and reduce CO_2 in to methanol, under visible light irradiation [15-18]. We proposed to couple both the wide bandgap TiO_2 and narrow bandgap $InVO_4$ semiconductors, so that it can facilitate for better charge carriers separation (see Figure 1 for band edge positions for both TiO_2 and $InVO_4$). In addition to the novel materials' development, it is also proposed to design a custom made reactor for the UV-Visible light photocatalysis for the generation of hydrocarbons from CO_2 and H_2O.

METHODS AND METHODOLOGY

The synthesis of TiO_2-Xwt.%$InVO_4$ nanocomposites will be carried out by an inexpensive high energy mechanochemical processes using planetary ball mill. Various optimization procedures will be adopted in terms of concentration of $InVO_4$, particle sizes of both TiO_2 and $InVO_4$, milling medium and duration of milling etc. to obtain the high yield material with maximum conversion efficiency. The as-synthesized nanocomposites will be extensively characterized using state-of-the-art analytical tools such XRD, SEM, EDAX, FTIR, UV-Vis and BET to explore the structural, microstructural, elemental, chemical and surface properties. Photocatalytic reactors will be designed and fabricated by optimizing the parameters such as power of light irradiation, amount of photocatalyst, concentration of source gases or initial contaminant, air flow, the time of irradiation etc.

TASKS AND MILESTONES

Task 1: Development of novel materials: In this task the base materials such as both plain TiO_2 and $InVO_4$ will be prepared by sol-gel synthesis route. In some instances, for better comparison, we will also examine the commercial TiO_2 (Degussa P-25 and/or Sigma Aldrich). After successful preparation of the precursor materials, we will synthesize the nanocomposite of TiO_2-Xwt.%$InVO_4$ by solid state mechanochemical milling under different experimental conditions. The major milestones in this task is to develop nanocomposites, that have an ability to generate more number of electron-hole pairs (EHP) and also extend their recombination rates so that they can participate in the photo-oxidation or photo-reduction processes efficiently under visible light.

Task 2: Development of photocatalytic reactor: In this task the team will work with the faculty mentor to design, fabricate and develop photocatalytic reactor (batch type or tubular configuration) and optimize the experimental parameters for yielding the maximum efficiency and throughput. The schematic diagram for the reactor design is given in the Figure 2. The major milestone to be achieved in this task is to successfully develop photocatalytic reactor that can be utilized to either decontaminate the water borne toxic (organic) chemicals such as phenol, azo dyes etc and also to generate hydrocarbon by photo-reducing reactions of CO_2 and H_2O.

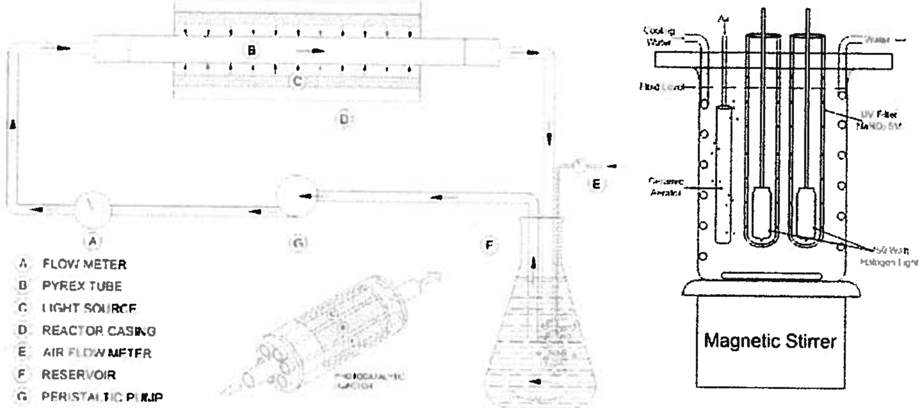

Figure 2: Schematics of Tubular and batch type photocatalytic reactors

PROJECT DELIVERABLES

Project deliverable in terms of quarterly and annual reports will be presented to the SPS and ΣΠΣ in periodic manner. The results and major accomplishments will be presented as either oral or poster presentations at the SPS, Sigma-Pi-Sigma,NSBP, AIP conferences. The results and the manuscript prepared from the project work will be communicated to the undergraduate research journals or proceedings for publications.

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BUDJET AND JUSTIFICATION

No.	Item Description	Proposed Budget (in dollars)	Justification or Remarks
1	**Chemicals** (Ti-Butoxide, Ti-Chloride solutions, Indium nitrate precursors, phenol, azo dyes), **Solvents** (solvents such as Isopropanol, Acetone, toluene, pentane etc.), **Acids** (Nitric and hydrochloric acid), **Bases** (Sodium hydroxide, Ammonium hydroxide)	800.00	To prepare TiO_2 and $InVO_4$ by chemical route using solvents, acids and bases. Once get the pure TiO_2 and $InVO_4$, we will try to mix in appropriate stoicheometry in planetary ball mill.
2	**Gases** (Ultra high pure nitrogen, compresses air, carbon dioxide, helium and hydrogen) and Liquid nitrogen	300.00	Gases will be used for both synthesis, & photocatalytic measurements
3	**Fabrication and design** of photocatalytic reactor	600.00	Glassware, temperature controllers, UV light bulbs, peristaltic pump, hot plates etc.
4	**Accessories for Characterization,** UV-Vis and FTIR spectrometer and BET surface area tool)	300.00	UV cuvets, eppendorf, syringes, KBr window glass & powder, Cotton wool, weighing boats.
	Total	**2000.00**	