

# Book of Abstracts



**Editors:**  
**Giovanni Hernández-Flores, Héctor M. Poggi-Varaldo,**  
**Omar Solorza-Feria**

**XV International Congress of the Mexican Hydrogen Society  
September 22 – 25, 2015  
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# **Book of Abstracts**

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## Preface

This book gathers the Abstracts of the 15<sup>th</sup> *International Congress of the Mexican Hydrogen Society (15IC MHS)* held in September 22-25, 2015, in the installations of the Center for Advanced Studies and Research (CINVESTAV), Mexico City, Mexico.

This book aims at reaching a wide audience including researchers, practitioners, managers, and students who aspire to learn about or to create a deeper scientific foundation for Hydrogen-based energies, design and engineering of fuel cells and other systems based on Hydrogen, and its management and innovation.

The 15IC MHS accepted a total of 144 abstracts (Table 1) after a strict peer-reviewing process. It is worth highlighting the increase of the contributions classified under the topics **Renewable energy systems** and **Nanostructured materials**, that constituted 18-19% each of the total abstracts and were close to the most classic and mature subject **Hydrogen production, storage and applications** (nearly 21%, Table 1). Biological hydrogen production, biorefineries, microbial fuel cells, nanomaterials for electrodes, membrane/separator design and testing, coupling solar energy to hydrogen production, are examples of emerging topics covered. Together, they make nearly half of the abstracts of the Congress.

Table 1. Distribution of abstracts per technical subject of the Congress

Subject	No. of Abstracts	Proportion (%)
<b>Hydrogen production, storage and applications</b>	30	20.83
<b>Direct oxidation fuel cells,</b>	10	6.94
<b>Fuel cells components and stacks</b>	21	14.58
<b>Modeling and design</b>	15	10.42
<b>Renewable energy systems</b>	26	18.06
<b>Control and power conditioning</b>	4	2.78
<b>Policies, economy and market strategies</b>	5	3.47
<b>Nanostructured materials</b>	27	18.75
<b>Environmental aspects</b>	4	2.78
<b>Miscellaneous</b>	2	1.39
<b>TOTAL</b>	144	100.00

This striking feature of the abstract distribution is consistent with the locomotive effect of Hydrogen on other Renewable Energies systems (via coupling, integration, preparation, etc.) as well as the use of Nanoscience-Nanotechnology approaches for designing and optimizing materials related to Hydrogen energy. Moreover, it is an indication of the high degree of innovation that characterizes Hydrogen energy R&D.

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The *15IC MHS* is also preparing the book “*Advances in Hydrogen Energy-2015*” whose chapters will be based on selected full articles presented in the Congress.

Therefore, this Book of Abstracts of the *15IC MHS* along with the book “*Advances in Hydrogen Energy-2015*” offer a body of the current cutting-edge approaches and knowledge in Hydrogen energy and will be a valuable tool in developing new strategies for fostering the Hydrogen energy new era.

We look forward to meeting you at the 16<sup>th</sup>. International Congress of the Mexican Hydrogen Society in 2016. Keep posted.

Professor Dr. Héctor M. Poggi-Varaldo  
Group Leader, Environmental Biotechnology and  
Renewable Energies R&D Group  
Dept. of Biotechnology and Bioengineering  
CINVESTAV del IPN, Mexico City, Mexico.



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## **Acknowledgements**

The Mexican Hydrogen Society and the Editors of this Book acknowledge the contribution of the following persons:

Mr. Jaime Borbolla-Gaxiola with the GBAER, DBB, CINVESTAV  
Ms. Miriam Tellez-Cruz with the FC&H2 Group, DQ, CINVESTAV  
Ms. Luz de María Bretón-Deval, M.Sc., with the GBAER, DBB, CINVESTAV  
Ms. Lilian Domínguez-Montero, B.S. Chem.Eng., with the GBAER, DCTS, CINVESTAV

Also, the effort and participation of the Reviewers in the peer-review process of the Abstracts is gratefully acknowledged:

Acuapan Hernández Javier – CINVESTAV-IPN  
Arriaga Gerardo– CIDETEQ  
Barbosa Pool Romeli – UQROO  
Benavides Cantú Roberto – CIQA  
Bretón Deval Luz de María – CINVESTAV-IPN  
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Fernández Valverde Suilma Marisela – ININ  
Fernández Villagómez Georgina – UNAM  
González Becerra Aldo E. – CSIC-CBM SEVERO OCHOA  
González García Gerardo – UACM  
González Huerta Rosa de Guadalupe – ESIQIE-IPN  
Hernández Melchor Dulce J. – UTTEC  
Hernández-Flores Giovanni – CINVESTAV-IPN  
Juárez López Katy – IBT-UNAM  
López Chávez Ernesto – UACM  
López Ortiz Alejandro – CIMAV  
Martínez Casillas Diana – UNIVERSIDAD DE BUENOS AIRES  
Matsumoto Kuwabara Yasuhiro – CINVESTAV-IPN  
Morales AcevedoArturo – CINVESTAV-IPN





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## **Hydrogen production, storage and applications**





**Use of Hydrogen for sustainable urban transport in Cuenca, Ecuador: a theoretical study**

**F. Posso<sup>a,\*</sup>; J. L. Espinoza<sup>a</sup>; J. Sánchez<sup>a</sup>; J. Zalamea<sup>b</sup>**

<sup>a</sup>Universidad de Cuenca. Av. 12 de Abril s/n y Agustín Cueva. Cuenca, Azuay. Ecuador

<sup>b</sup>CELEC EP. Hidropaute Business Unit. Panamericana Norte km 7, Cuenca, Azuay. Ecuador

**ABSTRACT**

The use of hydrogen in urban public transport in the city of Cuenca, Ecuador is analyzed by modeling and simulating the hydrogen production that would meet different levels of demand. This study proposes to use spilled turbinable energy, STE, to obtain H<sub>2</sub> via electrolysis due to the proximity of Cuenca to the Paute-Integral Hydroelectric Complex, which produces the largest amount of that available energy in Ecuador. STE is energy that could be generated from turbinable water that is spilled for diverse operational reasons. By combining the cost of excess electricity and the value billed to large consumers, it is possible to meet the energy demands of 100%, 50% and 10% of Cuenca's public bus fleet. This analysis determines the size of the electrolytic plant as well as the cost of hydrogen production, valued at 1.76 US\$/kg in the best-case scenario, which is comparatively less than the value obtained in other Latin American and European cities for the same end use. The cost of hydrogen production is 1.8 times the selling price of diesel in Ecuador but when compared to the price at which the State buys diesel on the international market, the results show that the cost of hydrogen is 0.63 times the cost of diesel. The study proves that the best economic scenario is to cover 100% of the energy demand of the bus fleet, though this proposal could be implemented in stages. Despite the potential for full coverage of the energy required, aspects related to both infrastructure and costs should be studied in depth and are not included in this analysis. For example, the location of the electrolysis plant, the storage system, the scheme of distribution and supply of H<sub>2</sub>, the optimal size of the fuel cell bus fleet and their associated costs, among others. This study concludes that hydrogen production from untapped hydropower and its use in Cuenca's urban transport is a niche opportunity for leading the country towards a Hydrogen Economy. The results also provide valuable information for the Ecuadorian State in its efforts to diversify the country's energy matrix into a sustainable development path.

**Keywords:** Hydrogen production, H<sub>2</sub>-FC buses, Cost model, Sustainable transport

\*Contact: Fausto Posso, Phone: (593) 990411328. Mail: fausto.posso@ucuenca.edu.ec



**Photobiological Hydrogen production by *Chlamydomonas* sp. and *Chlorella* sp.**

**E.M. Hernández-Hernández<sup>a</sup>; C.A. Cortés-Escobedo<sup>b\*</sup>**; R. Olvera-Ramírez<sup>a</sup>

<sup>a</sup>Escuela Nacional de Ciencias Biológicas-IPN, Prolongación de Carpio y Plan de Ayala, S/N, Casco de Santo Tomás, Miguel Hidalgo, México, D.F.

<sup>b</sup>Centro de Investigación e Innovación Tecnológica-IPN, Cda. CECATI S/N, Santa Catarina, Azcapotzalco, México D.F.

**ABSTRACT**

Energy generation currently has significant environmental impacts, an alternative to this problem are hydrogen technologies. It has been discovered that some green algae and cyanobacteria are able to generate molecular hydrogen (H<sub>2</sub>) photosynthetically, this process is called biophotolysis. The aim of this research was to evaluate the production of H<sub>2</sub> in mineral medium without sulfur in *Chlamydomonas* sp and *Chlorella* sp. cultures in suspension and immobilized in alginate.

Growth kinetics during cultivation in mineral medium BG-11, and the effect of immobilization on the cell growth are reported and discussed. Hydrogen production induction was tested in sulfur deprivation, anaerobic conditions and continuous light for 19 days by using a Differential Electrochemical Mass Spectrometer (DEMS) to identify hydrogen presence.

The gas samples analysis showed positive results for H<sub>2</sub> production in all the cultures, nevertheless the immobilization technique improved hydrogen production specially in *Chlamydomonas* sp. On the other hand, *Chlamydomonas* sp. immobilization influences on its growth rate but it does not affect the survival. Additionally *Chlamydomonas* sp. was more resistant to stress conditions than *Chlorella* sp. The use of immobilization technique facilitates organisms handling without affecting the production of hydrogen, so making necessary adjustments, the procedure for obtaining hydrogen on a photobioreactor can be scaled and coupled to fuel cells.

**Keywords:** Biohydrogen, Biophotolysis, Sulfur deprivation, *Chlamydomonas* sp, *Chlorella* sp.

\* Corresponding author:

Claudia Alicia Cortés Escobedo, 57296000 ext. 62311, Cerrada de Cecati S/N. Col. Santa Catarina Azcapotzalco México D. F. CP:02250, claudia.alicia.cortes@gmail.com

**Photocatalytic hydrogen production using Pd, Co and Ni oxides based on Au/TiO<sub>2</sub> catalysts**

**E. Albiter<sup>a</sup>; C. E. Barrios<sup>a</sup>; J. M. Gracia-Jiménez<sup>b</sup>; R. Zanella<sup>a,\*</sup>**

<sup>a</sup> Centro de Ciencias Aplicadas y Desarrollo Tecnológico - Universidad Nacional Autónoma de México, Ciudad Universitaria, Circuito Exterior s/n., Apdo. Postal 04510, Del.Coyoacán, Distrito Federal, México.

<sup>b</sup> Instituto de Física - Benemérita Universidad Autónoma de Puebla, Apdo. Postal J48, Col. San Manuel 72570- Puebla, México.

**ABSTRACT**

In the present work the photocatalytic production of hydrogen over Au/TiO<sub>2</sub> based photocatalysts was studied, using methanol as sacrificial agent (vol. ratio 20:180 CH<sub>3</sub>OH:H<sub>2</sub>O). Also, the effect of surface modification with Pd, Co and Ni oxides on the production of H<sub>2</sub> under UV light irradiation (~ 254 nm) was assessed. The metal oxides were first deposited on TiO<sub>2</sub> (Degussa P25) by incipient wetness impregnation followed by thermal treatment under H<sub>2</sub> (Pd and Co) or air (Ni). After that, Au was deposited by deposition-precipitation with urea (DPU) and then the catalysts were thermally activated at 300 °C under air atmosphere (Spatial Velocity = 2 g/ml.min).

The prepared photocatalyst were characterized by UV-Vis spectroscopy, photoluminescence (PL), EDS and HRTEM. The nominal metal content was ~ 0.5 wt. % and the Au:M<sub>x</sub>O<sub>y</sub> molar ratio was 1:1. The samples presented the characteristic UV absorption of TiO<sub>2</sub> and the absorption peak in the visible region associated with the surface plasmon absorption of Au nanoparticles (~ 550 nm). The (HR)TEM experiments showed that the metallic particles size was < 3 nm.

The Au-Pd oxide photocatalyst exhibited the highest H<sub>2</sub> production (5 mmol H<sub>2</sub>.g<sub>cat.</sub><sup>-1</sup>.h<sup>-1</sup>) because of palladium was able to maintain its metallic state and its ability to act as electron sink. The Au-Ni oxide and Au-Co oxide photocatalyst showed a similar performance (3.5 and 3mmol H<sub>2</sub>.g<sub>cat.</sub><sup>-1</sup>.h<sup>-1</sup>) compared to the Au/TiO<sub>2</sub> material (3.3 mmol H<sub>2</sub>.g<sub>cat.</sub><sup>-1</sup>.h<sup>-1</sup>) despite the fact that they had a smaller amount of Au. Probably, these oxides were working as promoter for water splitting reaction. The PL experiments showed that the presence of Au metal nanoparticles reduce the electron-hole recombination but also the presence of oxides in the Au-M<sub>x</sub>O<sub>y</sub> materials further enhance the charge separation, compared with Au/TiO<sub>2</sub> reference photocatalyst. The improved activity can be explained in terms of the enhanced charge separation observed in PL results, compared to the other materials the Au-Pd oxide photocatalyst showed the highest reduction in PL intensity signal..

**Keywords:** Hydrogen production, Water splitting, Au nanoparticles, TiO<sub>2</sub>

\* Corresponding author:

Rodolfo Zanella Specia, tel.+52 55 56228635; fax +52 55500654

rodolfo.zanella@ccadet.unam.mx



**Hydrogen production from methanol/water photocatalytic decomposition  
using Pt catalysts supported on hollow@TiO<sub>2</sub> core-shell nanostructures**

**O.F. Plascencia-Hernández<sup>a\*</sup>; G. Valverde-Aguilar<sup>a</sup>; M.A. Valenzuela<sup>b</sup>;  
Nicolás Cayetano-Castro<sup>c</sup>; Roberto Vazquez-Arreguín<sup>d</sup>**

<sup>a</sup>Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada Unidad Legaria del Instituto Politécnico Nacional

<sup>b</sup>Lab. Catálisis y Materiales. Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional. Zacatenco, 07738 México, D.F., México

<sup>c</sup>CNMN, Instituto Politécnico Nacional. Luis Enrique Erro s/n, U. Prof. Adolfo López Mateos, Gustavo A. Madero, 07738 Ciudad de México, Distrito Federal, México

<sup>d</sup>Instituto Politécnico Nacional- Escuela Superior de Cómputo, Av. Miguel Othón de Mendizábal s/n Col. La Escalera, Gustavo A. Madero, CP 07320, Distrito Federal, México

**ABSTRACT**

Global warming, the big problem of the 21th century, is caused by the increase in the concentration of greenhouse gases by the use of fossil fuels. Therefore, it is necessary to change the use of fossil fuels to carbon-free energies (carbon is the main greenhouse gas) such as H<sub>2</sub>, furthermore it should be obtained from a renewable source energy like solar energy. The development of materials that can transform solar energy toward chemical energy is vital to use Hydrogen as an energy carrier or fuel.

Core-shell structures exhibit interesting characteristics, like shield sensitive materials of the medium, or by tuning the band gap energy. In this work, core-shell structures were synthesized by a modified sol-gel method. The effect of Pt content (1-7 wt.%) and thermal treatments (500-900°C) on the photocatalytic activity were the main parameters studied. These materials exhibited an average size of 200 nm and a thickness-shell of 40 nm. The band gap energy remained still at the ultraviolet region, but one sample containing 7 wt.% Pt showed a slight blue shift. Samples calcined at 900°C were crystalline materials (anatase phase), and those calcined at lower temperatures were amorphous.

H<sub>2</sub> production was studied by using methanol as sacrificial electron donor in a methanol:water molar ratio of 1:5, and a 200 W Xenon lamp as irradiation source. The standard TiO<sub>2</sub> P25 Degussa was used as reference photocatalyst. The highest H<sub>2</sub> production yield was obtained with the 7 wt.% of Pt photocatalyst.

It was demonstrated that crystalline samples were photoactive to H<sub>2</sub> production compared with no activity of amorphous samples, which means that this property was significantly more important than Pt loading.

**Keywords:** Hydrogen production, Core-shell, Water splitting

\* Corresponding author: Address: Legaria 694, Colonia Irrigación, Miguel Hidalgo, 11500. Ciudad de México, Distrito Federal, México. Tel. (52 55) 57296000 ext. 67763, Fax (52 55) 53293255; E-mail: fernandoplascenciah@gmail.com



## **Hydrogenation and dehydrogenation in air-exposed Mg-Fe mixtures**

**K. Suárez-Alcántara<sup>a,\*</sup>; A. F. Palacios<sup>b</sup>; J. G. Cabañas-Moreno<sup>c</sup>**

<sup>a</sup> Unidad Morelia del Instituto de Investigaciones en Materiales de la Universidad Nacional Autónoma de México, Antigua carretera a Pátzcuaro 8701, Col. Ex-hacienda de San José de la Huerta, Morelia, Michoacán, 58190, México

<sup>b</sup> ESIME Zacatenco, Av. Luis Enrique Erro S/N, Unidad Profesional Adolfo López Mateos, Zacatenco, Delegación Gustavo A. Madero, Distrito Federal, 07738, México.

<sup>c</sup> Centro de Investigación y de Estudios Avanzados, IPN, Av. Instituto Politécnico Nacional 2508, México, D. F., 07360, México.

### **ABSTRACT**

Mg-Fe mixtures with a Fe content of 3 wt.% and 6 wt.%; here in-after Mg-Fe(3wt.%) and Mg-Fe(6wt.%), were produced by ball milling, exposed to air for 12 hours and tested in hydrogenation and dehydrogenation reactions. Despite the long accepted idea that oxidized Mg does not store hydrogen; hydrogen storage was proved. The H<sub>2</sub> uptake was 5.3 wt. %, 5.6 wt. % and 6.2 wt. % for air-exposed Mg, Mg-Fe(3wt.%) and Mg-Fe(6wt.%) mixtures respectively at 350°C and 30 bar. Fe addition had a beneficial influence on the kinetics and the hydrogen uptake and release compared to air-exposed Mg; partial hydrogen release was observed even at 250°C. From pressure-composition isotherm (PCI) experiments, the enthalpy and entropy of hydrogenation of air exposed Mg-Fe mixtures was  $\Delta H_{\text{abs}} = -62 \text{ kJ mol}^{-1} \text{ H}_2$  and  $\Delta S_{\text{abs}} = -117 \text{ J K}^{-1} \text{ mol}^{-1} \text{ H}_2$ . The values of entropy and enthalpy of the dehydrogenation reaction were found  $\Delta H_{\text{des}} = -74 \text{ kJ mol}^{-1} \text{ H}_2$  and  $\Delta S_{\text{des}} = -130 \text{ J K}^{-1} \text{ mol}^{-1} \text{ H}_2$  for the air exposed Mg-Fe mixtures. Powder X-ray diffraction of the studied materials confirmed the formation of fine mixtures. No evidence of formation of Mg<sub>2</sub>Fe or Mg<sub>2</sub>FeH<sub>6</sub> was found.

**Keywords:** Hydrogen storage, Air exposed magnesium, Mg-Fe mixtures

\* Corresponding author:

Karina Suárez Alcántara, +52 (55) 5623-7300 ext 80548

Email: karina\_suarez@iim.unam.mx

## **Dehydrogenation study of $\text{LiAlH}_4$**

**J. R. Tena-Garcia<sup>a</sup>; K. Suárez-Alcántara<sup>a,\*</sup>**

<sup>a</sup> Unidad Morelia del Instituto de Investigaciones en Materiales de la Universidad Nacional Autónoma de México, Antigua carretera a Pátzcuaro 8701, Col. Ex-hacienda de San José de la Huerta, Morelia, Michoacán, 58190, México

### **ABSTRACT**

$\text{LiAlH}_4$  is a high-promising  $\text{H}_2$  storage material; it stores up to 7.9 wt.% (for  $\text{H}_2$  storage applicability). The dehydrogenation reaction occurs well below  $150^\circ\text{C}$ . It is generally accepted that if a  $\text{H}_2$  storage material release hydrogen easily, the re-hydrogenation reaction will become more complicated. This is the case of  $\text{LiAlH}_4$ , where with the addition of suitable chemicals, dehydrogenation reaction has been observed to occur even during ball-milling or near room temperature. We present a dehydrogenation study of  $\text{LiAlH}_4$  mixed with  $\text{TiCl}_3$ ,  $\text{TiF}_3$ ,  $\text{CeO}_2$  and  $\text{PdCl}_2$ . The  $\text{LiAlH}_4$  + additive mixtures were prepared by ball-milling. The dehydrogenation reactions were performed in a Sieverts-type reactor heating up the samples to  $275^\circ\text{C}$  for complete dehydrogenation. As-milled and dehydrogenated materials were characterized by means of scanning electron microscopy (SEM), powder X-ray diffraction (P-XRD) and differential scanning calorimetry (DSC). Among the tested additives, the  $\text{TiCl}_3$  preserves better the  $\text{LiAlH}_4$  during ball-milling and keep a high quantity of stored hydrogen. The experimental evidence points to  $\text{TiCl}_3$  as a suitable candidate for further re-hydrogenation experiments.

**Keywords:** Hydrogen storage, Nanomaterials, Ball Milling

\* Corresponding author:

Karina Suárez Alcántara, +52 (55) 5623-7300 ext 80548

Email: karina\_suarez@iim.unam.mx



**On the dehydrogenation of 2LiBH<sub>4</sub>/Al mixture**

**J. L. Carrillo Bucio<sup>a</sup>; K. Suárez-Alcántara<sup>a,\*</sup>**

<sup>a</sup> Unidad Morelia del Instituto de Investigaciones en Materiales de la Universidad Nacional Autónoma de México, Antigua carretera a Pátzcuaro 8701, Col. Ex-hacienda de San José de la Huerta, Morelia, Michoacán, 58190, México

**ABSTRACT**

2LiBH<sub>4</sub>/Al + additives mixtures were prepared by ball milling; their dehydriding reactions were studied at 380°C and 5 bar hydrogen pressure. The dehydriding reactions were performed in a home-made Sieverts type reactor. The expected dehydrogenation products were a mixture of LiH and AlB<sub>2</sub>, with a H<sub>2</sub> storage capacity of 8.4 wt.%. The dehydrogenation reaction of the mixture without additives was slow and incomplete. Thus five additives were chosen to improve dehydrogenation reaction: TiF<sub>3</sub>, TiCl<sub>3</sub>, CeO<sub>2</sub>, Pd and PdCl<sub>2</sub>. As-milled materials and dehydrogenated materials were characterized by means of scanning electron microscopy (SEM), powder X-ray diffraction (P-XRD) and differential scanning calorimetry (DSC). Combined with hydrogenation studies of the LiH/AlB<sub>2</sub> mixture, it is intended to make the reaction  $2\text{LiH} + \text{AlB}_2 + 3\text{H}_2 \leftrightarrow 2\text{LiBH}_4 + \text{Al}$  completely reversible.

**Keywords:** Hydrogen storage, Borohydrides, Reactive hydride composites

\* Corresponding author:

Karina Suárez Alcántara, +52 (55) 5623-7300 ext 80548

Email: karina\_suarez@iim.unam.mx

**On the hydrogenation of 2LiH/AlB<sub>2</sub> mixture**

**D. Ayala Ayala<sup>a</sup>; K. Suárez-Alcántara<sup>a,\*</sup>**

<sup>a</sup> Unidad Morelia del Instituto de Investigaciones en Materiales de la Universidad Nacional Autónoma de México, Antigua carretera a Pátzcuaro 8701, Col. Ex-hacienda de San José de la Huerta, Morelia, Michoacán, 58190, México

**ABSTRACT**

2LiH/AlB<sub>2</sub> + additives mixtures were prepared by ball milling; their hydriding reactions were studied at 350°C and 43 bar hydrogen pressure. The expected hydrogenation products were a mixture of LiBH<sub>4</sub>+Al with a hydrogen storage capacity of 8.5 wt.%. The hydrogenation reaction of the mixture without additives was slow and not complete. Thus five additives were chosen to improve hydrogenation reaction: TiF<sub>3</sub>, TiCl<sub>3</sub>, CeO<sub>2</sub>, Pd and PdCl<sub>2</sub>. The additives covered a wide range of materials, from the typical additives for hydrogen storage to noble metals. CeO<sub>2</sub> additive produced the best results improving the hydrogenation reaction. As-milled materials and hydrogenated materials were characterized by means of scanning electron microscopy (SEM), powder X-ray diffraction (P-XRD) and differential scanning calorimetry (DSC).

**Keywords:** Hydrogen storage, Borohydrides, Reactive hydride composites

\* Corresponding author:

Karina Suárez Alcántara, +52 (55) 5623-7300 ext 80548

Email: karina\_suarez@iim.unam.mx

## **A novel production method of TiFeH<sub>x</sub>-Ni for hydrogen storage**

**J. C. Carranza-García<sup>a</sup>; K. Suárez-Alcantara<sup>a,\*</sup>; J. G. Cabañas-Moreno<sup>b</sup>**

<sup>a</sup> Unidad Morelia del Instituto de Investigaciones en Materiales de la Universidad Nacional Autónoma de México, Antigua carretera a Pátzcuaro 8701, Col. Ex-hacienda de San José de la Huerta, Morelia, Michoacán, 58190, México

<sup>b</sup> Centro de Investigación y de Estudios Avanzados, IPN, Av. Instituto Politécnico Nacional 2508, México, D. F., 07360, México.

### **ABSTRACT**

TiFe alloys have been studied as H<sub>2</sub> storage materials for stationary non-demanding applications. Several additives and partial metal replacement have been proposed to improve the hydrogenation/dehydrogenation characteristics of the TiFe alloy. The most used production method of the TiFe alloy in the hydrogenated form i.e. TiFeH<sub>x</sub>, is the TiFe alloy fabrication by meting of the elements, grinding until suitable particle size, activation for hydrogen storage and finally hydrogen exposure. Another method is the ball milling of the elements followed by activation and H<sub>2</sub> exposure.

As an alternative, in the present work we propose the production of the TiFeH<sub>x</sub> directly by reactive ball milling of a hydride and a metal:



Nickel with a load of 1 wt.% was added; then the TiFeH<sub>x</sub>-Ni was studied for hydrogen storage and characterized by means of scanning electron microscopy (SEM) and powder X-ray diffraction (P-XRD). After 50 hours of ball milling, SEM images show a homogeneous distribution of all the components of the alloy. P-XRD demonstrates the formation of TiFe and TiFeH<sub>2</sub> along peaks of unreacted TiH<sub>2</sub> and Fe. The as-milled material is already reactive for hydrogen release at room temperature, no activation process is needed. Hydrogen release quantification is under process by means of kinetic curves.

**Keywords:** Hydrogen storage, Nanomaterials, Reactive Ball Milling

\* Corresponding author:

Karina Suárez Alcantara, +52 (55) 5623-7300 ext 80548

Email: karina\_suarez@iim.unam.mx

**Photocatalytic hydrogen evolution on TiO<sub>2</sub>/HKUST-1  
composites under visible light**

**M.A. Valenzuela<sup>a</sup>; F.M. Martínez<sup>a</sup>; S. Alfaro<sup>a</sup>; A.L. Luna<sup>b</sup>; C. Colbeau-Justin<sup>b</sup>**

<sup>a</sup>Lab. Catálisis y Materiales. ESIQIE-Instituto Politécnico Nacional. Zacatenco, México D.F., México

<sup>b</sup>Laboratoire de Chimie Physique, CNRS UMR 8000 Université Paris-Sud, Bâtiment 349, 91405, Orsay CEDEX, France

**ABSTRACT**

The photocatalytic H<sub>2</sub> generation can be obtained essentially by two different approaches: i) photocatalytic water splitting, and ii) photocatalytic reforming of organics. The first method relates to the capability of water to be reduced and oxidized by reacting with photogenerated electrons and positive holes, during semiconductor irradiation, in presence of selected cocatalysts. The second approach is based on the ability of some organic species, named sacrificial agents, to donate electrons to the positive holes of the illuminated photocatalyst and to be oxidized generating protons ions, while the latter are reduced by photogenerated electrons forming hydrogen in presence of proper co-catalysts.

Glycerol is a sustainable compound that can be used for H<sub>2</sub> production by photocatalytic reactions. This reaction has been studied extensively; yet, the overall performance towards H<sub>2</sub> evolution is low and in many cases a high photocatalytic activity is only achieved with UV-light irradiation. For this reason, the search for new materials active and stable in the presence of sunlight is of great interest today.

In the present work, several TiO<sub>2</sub>/HKUST-1 (Basolite C300 or MOF-199) composites were prepared by mechanical milling and solvothermal methods. The characterization was done by thermal analysis (TGA), UV-VIS DRS, infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and time-resolved microwave conductivity (TRMC). The evaluation of the composites was performed in a batch reactor by using a glycerol-water mixture and irradiating with simulated solar light. The gaseous effluent was analyzed by gas chromatography.

The composites absorbed photons in the UV-Vis region and showed photocatalytic activity for hydrogen production under different operating conditions. H<sub>2</sub>, CO<sub>2</sub> and CH<sub>4</sub> were detected as the main reaction products which could indicate a complex set of reactions including the reduction of protons and mineralization/decomposition of glycerol. The highest H<sub>2</sub> yield was obtained with the TiO<sub>2</sub>/MOF composite (1:1 weight ratio). The stability of the composite was evaluated in 5 continuous reaction cycles (8h per cycle), showing a loss of the initial activity of 10%.

**Keywords:** Hydrogen production, Photocatalysis, TiO<sub>2</sub>-MOF composites, Visible light

\* Corresponding author: M.A. Valenzuela Address: IPN-ESIQIE. Ed.8, Zacatenco, 07738, México D.F., México. Tel:57296000 ext. 55112, E-mail: mavalenz@ipn.mx



**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Co-culture specific bacteria for hydrogen production in organic waste in different culture media**

**E. Avila-Vera<sup>a,b</sup>; D. Alcantara-Díaz<sup>c</sup>; G. Roa-Morales<sup>b</sup>; S.M. Fernandez-Valverde<sup>a\*</sup>**

<sup>a</sup>Depto. de Química, <sup>c</sup>Depto de Biología ININ, Apartado Postal 18-1027, México DF 11801, México, D.F.

<sup>b</sup>Depto de Posgrado, Facultad de Química, UAEMéx. Paseo Tollocan esq. Paseo colón, Toluca, México.

**ABSTRACT**

Fruit and vegetable waste (FVW) deposited in landfills contaminates air, land and underground water. A solution to this problem is the use of such waste as raw material for H<sub>2</sub> production. In order to utilize FVW it is necessary to determine its seasonal composition. Samples of FVW were obtained from Toluca's city market from November to December 2014. The samples were analyzed to determine proteins, fiber, fat and carbohydrates content. The carbohydrate percentage was  $6.7 \pm 0.3$ , equivalent to the  $6.4 \pm 0.5$  observed in samples collected between May to October, regardless of the season or kind of FVW in the mixture. An *Enterobacter cloacae* and *Clostridium butyricum* co-culture was used for H<sub>2</sub> production. The co-culture was grown in 1g of FVW (wet mass basis); 10 mL of growth medium (pH of 5.5) were mixed in 20 mL hermetically sealed glass bottles. L-cysteine or iron sulfate solutions were added and oxygen was displaced by a nitrogen gas current. Once the anaerobic conditions were established the bottles were heated for 20 minutes at 120 °C and allowed to reach room temperature, 2 drops of solution was taken and used for microorganism quantification, on a Petroff-Hausser chamber, and counted directly in a CARL ZEISS microscope. In the first place, the effect of L-cysteine or iron sulphate in phosphate solution on the growth *Clostridium butyricum* in the presence of FVW was assessed. L-cysteine alone inhibits bacterium growth until 80 h. In the case of iron sulfate, we observe rapid bacterial growth followed a marked decreased in growth after 25 h. Finally the bacterial number increases by 113% in 8 h when the media contains a mixture of iron sulfate and L-cysteine.

The results indicate that trace compounds added to the culture medium do not affect hydrogen production, as FVW provides sufficient carbon and nitrogen sources as well as micronutrients (i.e. iron) necessary for the bacterial metabolism. Additionally, there was no significant difference in bacterial growth rate with or without added compounds. Thus, FVW with no additional substances is sufficient as growth medium for co-cultures of the hydrogen-producing bacteria used in this study.

**Keywords:** Hydrogen production, Biohydrogen, Organic waste

\* Corresponding authors: Suilma M. Fernández Valverde, Evaristo Avila Vera.

Tel.: +525553297200 ext. 2277, Fax: +525553297301, e-mail address: evaristovae@yahoo.com.mx



## **Hydrogen production from compost leachates in an acidogenic SBR**

**S.I. Castro-Espinosa<sup>a</sup>; M. Meraz-Rodríguez<sup>b</sup>; C. Fajardo-Ortiz<sup>b,\*</sup>**

<sup>a</sup>Posgraduate student. Posgrado en Energía y Medio Ambiente, Divisiones de CBI y CBS.

<sup>b</sup>Department of Biotechnology, Universidad Autónoma Metropolitana-Iztapalapa, México D.F.

### **ABSTRACT**

Around 86,343,000 tons of garbage are produced daily in Mexico from which 50% correspond to the organic fraction composed by food and pruning wastes. This fraction is stabilized in composting plants and during this process a liquid effluent known as compost leachate is generated that may contain as high as 100 g COD/L and has been calculated that for 1000 tons of organic garbage, around 300 m<sup>3</sup> of leachate can be produced during a dry season. The huge amount of leachate makes difficult is proper management and disposition, remaining on the soil for long periods of time infiltrating in the soil and finally reaching the aquifers. The objective of this research was to treat the compost leachates in an acidogenic anaerobic process to obtain a biogas rich in H<sub>2</sub>.

A SBR was operated during 180 days in acidogenic conditions and was fed with compost leachates, obtained from the “Bordo Poniente” composting plant in Mexico City during February 2015. The organic loading rate was of 5.4 g COD/L, a pH of 5.0, an HRT of 1 day and in a sequence of 4 daily cycles of 6 hours each. The reactor was initially inoculated with an acidogenic acclimated sludge containing 6.6 g VS/L.

During the reactor operation, no organic matter removal was found and was transformed to VFA. The feeding contained 1.9 g COD-VFA/L and in the effluent 3.1 g COD-VFA/L were determined, corresponding to a VFA formation efficiency of 38% from the organic matter and the production of mainly propionic, butyric and valeric acids was detected. In contrast, no acetic acid production was found, probably due to the acidic conditions in the reactor that inhibited the acetogenesis of the VFA produced. The solubilization of volatile solids to VFA during the treatment was of 27%. The H<sub>2</sub> concentration in the biogas was of 95% with traces of CO<sub>2</sub> and CH<sub>4</sub>, for a productivity of 0.281 L H<sub>2</sub>/L<sub>reactor</sub>-d and aspecific hydrogenogenic activity of 0.213 L H<sub>2</sub>/g VS-d. The leachate treatment in the acidogenic SBR was successful for the H<sub>2</sub> production with productivity comparable to those reported for high strength effluents.

**Keywords:** Hydrogen production, Compost leachates, Acidogenic SBR

\* Carmen Fajardo Ortiz, (5255) 58044723; cfaj@xanum.uam.mx



**Photocatalytic hydrogen production with  $\text{TiO}_2\text{-Ni}_x\text{O}_y$  as mixed oxide**

**A. Pérez-Larios<sup>1,2,3,4\*</sup>; R. Gómez<sup>3</sup>; R. Zanella<sup>4</sup>**

<sup>1</sup>Universidad de Guadalajara, Centro Universitario de los Altos, Depto. Ciencias Biologicas, Carretera a Yahualica km. 7.5, Tepatitlán de Morelos, Jalisco, México. 47600.

<sup>2</sup>Instituto Tecnológico Superior de Arandas, Depto. Ing. Ambiental, Libramiento Sur km 2.7 carretera Arandas-León, Arandas, Jalisco, México. 47180.

<sup>3</sup>Universidad Autónoma Metropolitana-Iztapalapa, Depto. de Química, Área de Catálisis, Av. San Rafael Atlixco No 189, 09340, D.F. México.

<sup>4</sup>Centro de Ciencias Aplicadas y Desarrollo Tecnológico, Universidad Nacional Autónoma de México (UNAM), 04510, Ciudad Universitaria, D.F. México.

**ABSTRACT**

The conversion of commercial fuels like hydrocarbon and alcohol to  $\text{H}_2$  can be achieved by catalytic chemical reactions such as steam reforming, partial oxidation and autothermal reforming. In general alcohol fuels like methanol and ethanol are more reactive than hydrocarbon fuels for steam reforming and are thus converted to  $\text{H}_2$  at lower temperature ranges than the cases of hydrocarbon reforming which occurs above 700 °C. Nanomaterials have been shown to behave quite differently from their bulk counterparts due to the effect of their quantumconfinement imposed upon the charge carriers. Since the photo-induced decomposition of water on  $\text{TiO}_2$  electrodes was discovered by Fujishima and Honda, titania-mediated semiconductor photocatalyst has attracted extensive interest towards the process of splitting of water into  $\text{H}_2$  and  $\text{O}_2$  with the use of sunlight due to their low cost method of hydrogen production.

The nanostructured materials of  $\text{TiO}_2$  and  $\text{TiO}_2\text{-Ni}_x\text{O}_y$  (metal load: 1.0, 3.0, 5.0 and 10 wt. %) samples were prepared by the sol-gel method followed by an annealing thermal treatment. The semiconductors were characterized by the BET, FT-IR, RAMAN, UV-vis and X-Ray techniques.

The X-ray diffractogram shows the characteristic peaks of anatase phase of  $\text{TiO}_2$ . The energy band gap for all mixed oxide materials are below the 3.2 eV. Shows the effects of Ni content as a displacement in the increases the doping metal, which suggests that is into the titania, the content with 1% of Ni showed better activity of approximately 8,000  $\mu\text{mol/h}$ . The results showed that the  $\text{H}_2$  production is a good alternative as fuel energy, using water splitting process.

**Keywords:** Hydrogen production, Nanomaterials, Photocatalysis, Mixed oxide

\* Corresponding author:

Alejandro Perez-Larios, 52-378-7828033, 47600; alex.perez.larios@gmail.com



**Improved hydrogen production by pretreating a solids stream derived from an OFMSW biorefinery**

**L. Romero-Cedillo<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>; T. Ponce-Noyola<sup>a</sup>; E. Ríos-Leal<sup>a</sup>;  
A.C. Ramos-Valdivia<sup>a</sup>; C.M. Cerda-García Rojas<sup>b</sup>; J. Tapia-Ramírez<sup>c</sup>**

<sup>a</sup>Departament of Biotechnology and Bioengineering, Environmental Biotechnology and Renewable Energy Group, Cinvestav-IPN, México, D.F.

<sup>b</sup>Departament of Chemistry, Cinvestav-IPN, México, D.F.

<sup>c</sup>Departament of Genetics and Molecular Biology, Cinvestav-IPN, México, D.F.

**ABSTRACT**

Due to the high availability of organic wastes generated in Mexico (28 million of tons/year), renewable energy from municipal solid waste (OFMSW) becomes an attractive and sustainable alternative that could compete with fossil energy. These wastes are made up 75% of carbohydrates and represent an economic source of raw materials that are mainly used in anaerobic digestion. This process is one of the initial steps in the HMZS biorefinery, in which hydrogen and methane are obtained. In later stages, namely enzyme production (Z) and saccharification (S), our biorefinery produce hollocelulases and saccarified liquors that could be used for either ethanol production or synthesis of added-value bioproducts. However, in stage Z, the waste solids stream Xz still has an acceptable contents cellulose ( $\approx 30\%$ ), although likely in its crystalline form that impairs further cellulose degradation. Therefore, pretreatments have been used to increase cellulose degradation and/or decrease lignin contents of a given lignocellulosic substrate. In this work, we applied two alkaline pretreatments ( $\text{Na}_2\text{CO}_3$  1M and  $\text{NaOH}$  1M) and one dilute acid treatment ( $\text{HCl}$  1.5% v/v) in order to increase cellulose accesibility with the goal to increase biohydrogen production in an H-M-Z-S biorefinery. We found that pretreatment with alkali  $\text{NaOH}$  1M, increased availability of cellulose by 30% of Xz compared to the non-pretreated materialsame residue not pretreated (39.6% and 29.7%, respectively). Pretreated residue Xz was fed to batch, biohydrogen-generating reactors either as the only feedstock or mixed with OFMSW. A remarkable additional biohydrogen production was observed. We conclude that pretreatment of the intermediate stream of solids Xz leads to a significant increase of biohydrogen generation in our biorefinery approach.

**Keywords:** Biohydrogen, Biorefinery, Cellulose, OFMSW, Pretreatment

\* Corresponding author:

Héctor M. Poggi-Varaldo, Phone number: 5747-3800 Ext. 4321& 4324, fax number: 5747-7002, Av. Instituto Politécnico Nacional #2508 Col. San Pedro Zacatenco, México, D.F. C.P. 07360; E-mail: r4cepe@yahoo.com



**Photoelectrocatalysis hydrogen production by Au, Pt doped TiO<sub>2</sub>**

**A. Martínez<sup>a,b</sup>; R. Rangel<sup>a,b</sup>; A. Dominguez – Gonzalez<sup>a</sup>; K. Esquivel<sup>a</sup>; E. Elizalde<sup>a</sup>; S.M. Durón – Torres<sup>b</sup>; C. Guzmán<sup>a,b\*</sup>**

<sup>a</sup>Facultad de Ingeniería, Universidad Autónoma de Querétaro, Cerro de las Campanas, C.P. 76000, Santiago de Querétaro, Qro., México.

<sup>b</sup>UACQ – UAZ, CU Siglo XXI Edificio 6, Km 6 Carr. Zac – Gdl, La Escondida Zacatecas, Zac, C.P. 96160, México.

**ABSTRACT**

Photoelectrochemical H<sub>2</sub> production is a promising alternative, however, the semiconductors materials (TiO<sub>2</sub>) is active only under UV radiation related with the band gap size (3.0 eV rutile, 3.2 eV anatase). One approach to reduce the band gap is doping TiO<sub>2</sub>. This method would substitute Ti<sup>4+</sup> ion or O<sup>2-</sup> ion into the TiO<sub>2</sub> lattice, forming intraband states, which could favor the visible light absorption of material.

Earlier studies shown that adding a noble metal in the TiO<sub>2</sub> lattice, such as Pt, Pd, Au, Ag; etc, improves significantly the photocatalytic activity of TiO<sub>2</sub>. This behavior could be explained by the action of novel metal as photogenerated electron acceptor. The electron can quickly transfer from the TiO<sub>2</sub> surface to the metal particle, leading to electron – hole separation and resulting in the improvement of photocatalytic efficiency. With this kind of modification is possible to produce more quantity of H<sub>2</sub> than the produced by photocatalyst. In this work, we have investigated the effect of the synthesis of TiO<sub>2</sub> - Pt and TiO<sub>2</sub> - Au introduced into a photoelectrochemical electrolyser, obtaining high H<sub>2</sub> production, than the obtaining with TiO<sub>2</sub>. This result is promising in order to be used like a hydrogen production process.

**Keywords:** Hydrogen production, Photoelectrochemical, Titanium dioxide, Platinum, Gold

\* Corresponding author:

Carlos Guzmán Martínez, (449) 1648652, C.P. 76000, e – mail: cgm1909@hotmail.com

**Evaluation of microorganisms settling ability in hydrogen production**

**C. E. Hernández-Mendoza<sup>a,b\*</sup>; G. Buitrón<sup>b</sup>**

<sup>a</sup>Institute of Ecology, Universidad del Mar. Ciudad Universitaria S/N, Puerto Ángel, Distrito de San Pedro Pochutla, Oaxaca, 70902, México.

<sup>b</sup>Laboratory for Research on Advanced Processes for Water Treatment, Instituto de Ingeniería, Campus Juriquilla, Universidad Nacional Autónoma de México. Blvd. Juriquilla 3001, Juriquilla, Querétaro, 76230, Mexico.

**ABSTRACT**

It was reported that microorganisms that do not settle after a settling time of 3 h in a sequencing batch reactor (SBR) may have a higher specific- $H_2$  production than those who settle. This finding has important consequences in the design and operation of the  $H_2$ -producing bioreactors. The objective of this paper was to evaluate the influence of the biomass settling ability in  $H_2$  production by biochemical  $H_2$  production (BHP) tests.

Anaerobic sludge was acclimated in a SBR to produce  $H_2$ . When biomass reached steady-state the biomass separation into settleable and non-settleable was done. To do this, the settling time was increased from 30 min to 3 h. The BHP tests were done in serum bottles inoculated with settled or non-settled biomasses. The operational conditions applied in the SBR were maintained in the BHP tests. Data were adjusted to the modified Gompertz equation.

The biogas production by the non-settleable biomass was significantly higher (ANOVA,  $\alpha=0.05$ ) than the biogas produced by the settled biomass. However, the  $H_2$  content in the biogas produced by the non-settled biomass was lower than in the one produced by the settled biomass. The specific-hydrogen production rates of the settled and non-settled biomasses were  $26 \pm 4 \text{ mL}_{H_2} \text{ g}_{VSS}^{-1} \text{ h}^{-1}$  and  $7 \pm 2 \text{ mL}_{H_2} \text{ g}_{VSS}^{-1} \text{ h}^{-1}$ , respectively. The non-settled biomass showed a dispersed growth pattern while the settled biomass had a floccular growth pattern. Both biomasses had a similar diversity (Jaccard diversity index = 0.9). Nonetheless, the differences in the relative abundances of some phylotypes, evaluated through the DGGE gel's band intensity, resulted in different microbial communities.

The influence of the biomass settling ability in hydrogen production was evaluated and it was found that the biomass that were able to settle had a higher hydrogen-specific production than the biomass that didn't settle.

**Keywords:** Hydrogen production, SBR, Settling, DGGE

\* Corresponding author:

Tel. +52(958)5843049 Ext. 113, E-mail: ceduardo.hernandez@gmail.com



**Kinetic study of hydrogen storage in calcium oxide**

**T. Ramírez-Rodríguez<sup>a\*</sup>; F. L. Castillo-Alvarado<sup>a</sup>**

<sup>a</sup>Instituto Politécnico Nacional, Av. Instituto Politécnico Nacional s/n, San Pedro Zacatenco, Gustavo A. Madero, D.F, México, 07738.

**ABSTRACT**

Studies from mechanical, thermodynamic and, kinetic parameters have been reported about H<sub>2</sub> storage. Extrapolation of energy carried by the variation of energy of a single point as a function of radial distance from the H<sub>2</sub> molecule from center of H<sub>2</sub> adsorption system to the outer surface has been used to locate the position where hydrogen molecules are adsorbed in the chemical system. The kinetic stability plays a very important role for hydrogen storage efficient, which is theoretically related to the energy gap of HOMO-LUMO. This work show the kinetic behavior of the molecule of calcium oxide which having a meso-porous structure that facilitates access to the entire surface of the particle of CaO, to optimize the structure of the adsorbent have been exceeded speed limits and extension in CO<sub>2</sub> capture, knowing that biomass represents a clean and removable resource for sustainable production of H<sub>2</sub>, based on steam gasification process, when combined with CO<sub>2</sub> capture.

The reactivity of CaO to capture CO<sub>2</sub>, where CaO involves, such as surface area, pore volume and pore size distribution of the CO<sub>2</sub> reactivity. The synthesis of tailored CaO for in situ CO<sub>2</sub> capture has not been attempted. There is also likely to be an optimal pore size range for CO<sub>2</sub> capture that does not limit access to unreacted CaO due the higher molar volume of CaCO<sub>3</sub> (36.9 cm<sup>3</sup> mol<sup>-1</sup>) compared to CaO (16.9 cm<sup>3</sup> mol<sup>-1</sup>). Gupta and Fan (2002) demonstrated enhanced CO<sub>2</sub> capture using CaO derived from precipitated CaCO<sub>3</sub> with pores predominantly in the meso-porous range (2-50nm) compared to naturally occurring limestone with pores in the micro-porous range (<2 nm). Carbonation was conducted at 650°C in 100% CO<sub>2</sub> in theory. The calculation of the energy required for the surface of the calcium oxide capture CO<sub>2</sub> and H<sub>2</sub> has been investigated in this work by Density Functional Theory Electronic Structure Program.

**Keywords:** Hydrogen production, CO<sub>2</sub> capture, DFT, Kinetic parameters

\* Teresa Ramírez-Rodríguez, 044 55 43520891, [teresa.ramirez7715@gmail.com](mailto:teresa.ramirez7715@gmail.com)

**New catalytic technology implementation on the  
hydrogen production industry**

**J. Fortuna-Espinosa**

**ABSTRACT**

Presenting a real case, where it was possible to implement a new catalytic technology for  $H_2$  production at industrial level, in a SMR (Steam Methane Reforming) plant type. Details relating to the technical and commercial part are presented, and the approach related to the economic benefits to be obtained by using this new technology. At the end, the final tests and results are shown from a technical and commercial perspective.

**Keywords:** Industrial application, New catalytic technology, Hydrogen Production

\* Corresponding author:

Total Energy, Consultoría en Hidrogeno,  
Guillermo Ortega Vargas, Manzana 3, Lote 25, Casa 4,  
Fraccionamiento Los Héroes 2ª Sección,  
Toluca, Estado de México, C.P. 50246  
Tel: 722 1995108, fax 722 1995108, [javier.fortuna@totalenergyh2.com](mailto:javier.fortuna@totalenergyh2.com)



## **A screening of hydrogen evolution during photocatalytic CO<sub>2</sub> reduction**

**M.P. Vázquez<sup>1,2,\*</sup>; M.A. Valenzuela<sup>1</sup>; J. Aguilar<sup>2</sup>; A.L. Luna<sup>3</sup>; C.Colbeau-Justin<sup>3</sup>**

<sup>1</sup> Lab. Catálisis y Materiales. ESIQIE-Instituto Politécnico Nacional. Zacatenco, México D.F., México

<sup>2</sup> Dpto. Estado Sólido. ESFM- Instituto Politécnico Nacional. Zacatenco, México D.F., México

<sup>3</sup> Laboratoire de Chimie Physique, CNRS UMR 8000 Université Paris-Sud, Bâtiment 349, 91405, Orsay CEDEX, France

### **ABSTRACT**

In the last decade, it has been a rebirth of the study of water splitting and photoreduction of CO<sub>2</sub> with the aim of producing solar fuels. This is a concept known as artificial photosynthesis, where sunlight is harvested and the energy is used to chemically convert water and carbon dioxide into fuels. It is worth noting that the activation and transformation of CO<sub>2</sub> into organic products is not an easy task, due to its thermodynamic stability and kinetic limitations. In particular, the photocatalytic reduction of CO<sub>2</sub> takes place by light absorption of the semiconductor, separation of the photo-generated charges, transportation to the surface and the catalytic reactions of oxidation and reduction with electrons and holes, respectively. However, a low photo-conversion efficiency and lack of selectivity to a single product are achieved attributed to the high reduction potential of CO<sub>2</sub> activation and the use of water as sacrificial reducing agent, since H<sub>2</sub>O can compete favorably for the electrons and produce preferentially hydrogen. This work has been focused to the study of the photocatalytic reduction of CO<sub>2</sub> by using different types of catalytic materials to know the effect on selectivity under the same operating conditions. Several oxides materials including metal and metal oxides supported on TiO<sub>2</sub>, ZnO, Ga<sub>2</sub>O<sub>3</sub> as well as mixed oxides and hybrid as CuO/TiO<sub>2</sub> (2.81 μmol/gr<sub>cat-h</sub>), CuO/Ga<sub>2</sub>O<sub>3</sub> (0.85 μmol/gr<sub>cat-h</sub>), Ag<sub>2</sub>O/ZnO (1.1 μmol/gr<sub>cat-h</sub>), Ag/TiO<sub>2</sub> (0.12 μmol/gr<sub>cat-h</sub>), Au/TiO<sub>2</sub> (0.78 μmol/gr<sub>cat-h</sub>), Au-Cu/TiO<sub>2</sub> (0.65 μmol/gr<sub>cat-h</sub>), as TiO<sub>2</sub>/MOFs (0.22 μmol/gr<sub>cat-h</sub>). These compounds were prepared and characterized by UV-Vis diffuse reflectance and time-resolved microwave conductivity, among others. These catalytic materials were evaluated under the same reaction conditions in the CO<sub>2</sub> photoreduction by using a glass cell with an aqueous solution of 30 %v NaOH/70%v isopropanol with simulated solar light (50 W). The gas effluent was analyzed by gas chromatography and the main detected products were hydrogen and methane. In general, all catalysts were active and selective to produce hydrogen and methane, however, the higher hydrogen yield was found with the CuO/TiO<sub>2</sub> materials and the highest selectivity to methane was obtained with the CuO/ZnO catalyst. The characterization results showed a clear influence of the chemical composition, structure, morphology, etc., of the different catalytic materials on the charge-carrier dynamics after excitation with light, which could explain the photocatalytic efficiency and selectivity.

**Keywords:** Photocatalysis, Hydrogen production, CO<sub>2</sub> reduction

\* Corresponding author: María Patricia Vázquez Romero; Tel. 52 553992770  
pvazquez@infinitum.com.mx



**Assembly and characterization of a PEM electrolyser for hydrogen generation from wave power**

**D. Moreno Antonio<sup>a,b</sup>\*; R. Sánchez Dirzo<sup>a</sup>; R. de G. González Huerta<sup>b</sup>**

<sup>a</sup>UNAM, FES-Zaragoza, Batalla e de Mayo, Col. Ejército de Oriente C.P. 09230, México D.F

<sup>b</sup>ESIQIE IPN, Laboratorio de Electroquímica y Corrosión, UPALM, C.P. 07738, México D.F.

**ABSTRACT**

The world is now facing enormous challenges associated with pollution, emissions of greenhouse gases, climate change and the need for sustainable development. The production of H<sub>2</sub> from renewable energy sources has the potential to bring a local energy solution through the electrolysis of water. A PEM electrolyser can produce H<sub>2</sub> continuously by converting electrical energy into chemical energy without any purification process and is one of the most important electrochemical energy-related processes.

The "BlowJet" is a wave energy conversion (WEC) device, which is currently being tested in a wave flume. The purpose of this device is to concentrate the energy of a wave train and offer it in a form more readily available as a jet that is capable of powering a turbine generator. A current pulse is generated with a specific voltage and amperage (1.5-2 V and 0.05-0.3 A). A PEM electrolyser performance depends mainly on the structure and electrochemical characteristics of the membrane electrodes assembly (MEAs). In this work different MEAs were analyzed using as the cathode platinum catalyst in a concentration of 0.3 mg/cm<sup>2</sup> and the RuO<sub>2</sub> and IrO<sub>2</sub> in the anode with concentrations of 4.5 mg/cm<sup>2</sup> and 1.5 mg/cm<sup>2</sup> respectively. Before each preparation of MEA, the Nafion 115 membrane is chemically activated with hydrogen peroxide and sulfuric acid using standard methodology. Before spraying, the membranes were dried and flattened. The variables were: number of catalyst and hot pressing conditions 5 tons and 120 ° C. Performance curves were obtained and compared with commercial device, thereby reducing the ohmic resistance of the MEA, and equating the commercial device.

**Keywords:** Electrolysis, Hydrogen production, PEM electrolyzers, Blowjet

\* Corresponding author:

David Alberto Moreno Antonio, cell: 044-55-47582875 home: 01 55 16437636,

Email: davidmorenoantonio@hotmail.com

**TiO<sub>2</sub> nanotubes array sensitized with CdS and Sb<sub>2</sub>S<sub>3</sub>, for  
photoelectrochemical hydrogen generation**

**J. E. Carrera-Crespo<sup>a\*</sup>; G. Ramos-Sánchez<sup>a</sup>; V. De la Luz<sup>a</sup>; F. González<sup>b</sup>;  
E. Barrera<sup>b</sup>; I. González<sup>a</sup>**

Universidad Autónoma Metropolitana-Iztapalapa. (<sup>a</sup>)Departamento de Química. (<sup>b</sup>)Departamento de IPH.  
Av. San Rafael Atlixco No. 186, C. P. 09340. Ciudad de México, Distrito Federal.

**ABSTRACT**

Photoelectrochemical H<sub>2</sub> production is currently being considered as a potential clean and renewable route for energy generation. TiO<sub>2</sub> nanotube arrays (TNAs) are interesting photoanodes with potential use in photoelectrochemical cells for H<sub>2</sub> production. Due to its 1D geometry, the recombination processes is diminished while the electron transport is accelerated toward the counter electrode, where they are subsequently scavenged by hydrogen ions on Pt cathode forming hydrogen gas. Moreover, the low fabrication cost, chemical stability, high specific surface area, photosensitivity, and catalytic potential, make TNA's valuable as photocatalytic and photoelectrocatalytic supports. However, the optical absorption range of TiO<sub>2</sub> (<387 nm) limits its practical use. Sensitization with narrower band gap semiconductors has been attempted to improve the photoresponse of TNAs in the visible region. In this work, we propose TNAs sensitization with CdS and Sb<sub>2</sub>S<sub>3</sub> nanoparticles, employing an electrochemical/thermal/chemical method, in order to improve the photoelectrochemical performance of TNAs and its use in photoelectrochemical cells for hydrogen production. TNAs sensitized with CdS and Sb<sub>2</sub>S<sub>3</sub> (Sb<sub>2</sub>S<sub>3</sub>/CdS/TNAs) were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), electrochemical impedance spectroscopy (EIS) and UV-Vis diffuse reflectance absorption spectra (DRS). We also investigated the photoelectrochemical behavior of the Sb<sub>2</sub>S<sub>3</sub>/CdS/TNAs photoelectrodes in a conventional three-electrode cell, and their H<sub>2</sub> production capacity in a H-type photoelectrochemical cell using a platinum plate as counter electrode. The Sb<sub>2</sub>S<sub>3</sub>/CdS/TNAs photoelectrodes showed a significant increase in H<sub>2</sub> production, compared with TNAs, Sb<sub>2</sub>S<sub>3</sub>/TNAs and CdS/TNAs photoelectrodes.

**Keywords:** Photoelectrochemical hydrogen production, Electrochemical/thermal/chemical method, Sb<sub>2</sub>S<sub>3</sub>/CdS/TNAs Bphotoanodes

\* Corresponding author:

J. E. Carrera-Crespo, (+52)5558044671 ext. 13, edgarcrespo@xanum.uam.mx



**$W_{1-x}Mo_xO_3 \cdot 0.33H_2O$  compounds synthesized by hydrothermal and microwave-radiation for  $H_2$  production**

**A. Arzola-Rubio; J. Camarillo-Cisneros; V. Collins-Martínez\***

Centro de Investigación en Materiales Avanzados S. C., CIMAV. Miguel de Cervantes 120, Chihuahua, Chih. México. CP 311136.

**ABSTRACT**

$WO_3$  has been thoroughly investigated and optimized to deliver high single wavelength quantum efficiencies [1, 2]. Unfortunately the stability of this oxide in aqueous environments, aided by an energetically low valence band which is defined largely by O 2p energy levels, also brings a large band gap which renders these materials transparent to most of the incident solar illumination. A series of hydrated Tungsten-Molybdenum oxides have been synthesized by hydrothermal and microwave radiation techniques. In both cases the  $WO_3 \cdot 0.33H_2O$  crystal lattice can be substituted with up to 75% Mo without structural alterations of the orthorhombic host structure. These products have a band gap suited at the visible range ( $\sim 2.00$  eV). Experimental data were explained by means of first-principle calculations in the framework of DFT and DFT+U; indirect semiconductors were obtained. Both compounds were evaluated for  $H_2$  production..

**Keywords:**  $H_2$  production; Water splitting; W/Mo solid solutions; DFT simulation

\* Corresponding author:

Virginia Collins Martinez, phone: +526144391129; e-mail: virginia.collins@cimav.edu.mx

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**Quantum yield for hydrogen production in photocatalytic water splitting  
using TiO<sub>2</sub>-Pt prepared by different methodologies**

**A. Calzada Hernández<sup>a</sup>; F. Orozco<sup>a</sup>; F. Guayaquil<sup>b</sup>; S. Escobedo<sup>b</sup>; C. Guzman<sup>a</sup>;  
H. de Lasa<sup>b</sup>; B. Serrano Rosales<sup>a\*</sup>**

<sup>a</sup>Universidad Autonoma de Zacatecas, Maestria en Ciencias de la Ingeniería, Zacatecas, México.

<sup>b</sup>Western University, Faculty of Engineering, Chemical Reactor Engineering Centre (CREC), London, ON, Canada.

**ABSTRACT**

The present study reports quantum yield calculations for H<sub>2</sub> production using a Pt modified titanium dioxide in a slurry medium, under near-UV irradiation, during the photocatalytic water splitting. The photocatalyst was prepared using three different methods: incipient wetness, wet impregnation and sol-gel. The catalysts were characterized by BET, X-ray diffraction, diffuse reflectance to obtain surface area, crystalline phases and the energy of band gap respectively. The results show that the photocatalysts by sol-gel have a greater surface area and crystal size smaller unlike the other two catalysts, and the three types of catalysts have a dominant anatase crystalline phase and a decrease of the band gap. Experiments were performed in a Photo CREC Water II Reactor adapted with a hermetic tank without air and using argon instead as carrier, with a photocatalyst load of 0.15 g/L and acid medium (pH=4.0). Regarding H<sub>2</sub> formation via H<sup>•</sup> free radicals, the addition of a 2 vol.% ethanol scavenger allowed to achieve significant amounts of H<sub>2</sub>. It was observed that the same amount of hydrogen was obtained after six hours of experiment with the catalyst prepared with sol-gel, wet impregnation and eventually with incipient wetness. However, the most important point is that the calculated values of the quantum yields are different for the three photocatalysts, with the highest value for the experiment with sol-gel photocatalyst, showing good degree of photon utilization and confirming the utility of the Pt modified TiO<sub>2</sub> photocatalyst and Photo CREC Water II Unit set up for the H<sub>2</sub> production, via water splitting.

**Keywords:** Hydrogen production, Photocatalysis, Quantum yield, Photo CREC reactor

\* Corresponding author:

B. Serrano Rosales, 52-492-9256690, ext 4668, beniser@prodigy.net.mx

## **Hydrogen storage of Mg nanoparticles confined in carbon cryogels**

**C. N. Vargas-Hernández<sup>a,\*</sup>; J. G. Cabañas-Moreno<sup>a</sup>; O. Solorza-Feria<sup>a</sup>;  
D. Bahena-Uribe<sup>a</sup>; T. L. Mercado-Castillo<sup>c</sup>; J. C. Garcia-Mayorga<sup>d</sup>; E. Reguera-Ruiz<sup>b</sup>**

<sup>a</sup>Centro de Investigación y Estudios Avanzados del IPN, Av. IPN 2508 Col. San Pedro Zacatenco, A. Postal 14-740, 07360 México D.F.

<sup>b</sup>Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada del IPN, Legaria 694 Col. Irrigación, 11500 México D.F.

<sup>c</sup>Escuela Superior de Ingeniería Química e Industrias Extractivas, U. Prof. Adolfo López Mateos Col. San Pedro Zacatenco, 07360 México D.F.

<sup>d</sup>Universidad Tecnológica de Tecamac, Carretera Federal México - Pachuca Km 37.5., Sierra Hermosa, 55740 Méx.

### **ABSTRACT**

Some theoretical studies predict that thermodynamic stability of  $\text{MgH}_2$  would be decreased in the form of nanoparticles or clusters. In addition, nanosized Mg exhibit other advantages derived from their small size: increased surface area, shortened hydrogen diffusion distances, increased number of grain boundaries to enhance hydrogen diffusion rates. However, Mg nanoparticles tend to grow or aggregate into large particles at high temperatures (573 K) during the hydrogen absorption and desorption cycles. In order to control the particle size distribution and efficiently prevent nanoparticles from coarsening or aggregating, a 'nanoconfinement' method is introduced to prepare nanosized Mg, for which nanoparticles are confined in a nanoporous scaffold material.

In our work, we have chosen nanoconfinement within porous carbon cryogels as a means to altering the thermodynamics and dehydrogenation kinetics of magnesium hydride. A wet impregnation method has been developed which involves reduction of magnesium acetylacetonate with sodium borohydride. The size of the Mg is directly influenced by the pore size of the carbon cryogels and can be varied from 5 to 20 nm. The optimized preparation method and the sorption properties of Mg-base hydrogen storage materials will be presented in this work.

**Keywords:** Hydrogen storage, Nanomaterials, Nanoconfinement, Carbon cryogels

\* Corresponding author:

C.N. Vargas Hernandez, México D.F., claudianvh@hotmail.com



**Effect of the neodymium addition to Rh on alumina supported catalysts  
in the activity and selectivity to hydrogen on CH<sub>4</sub> dehydrogenation**

**M. Caballero Diaz<sup>a,\*</sup>; G. Del Angel Montes<sup>a</sup>; A. Bonilla Sánchez<sup>a</sup>; D. Monroy Hernández<sup>a</sup>; I. Rangel<sup>a</sup>**

<sup>a</sup> Departamento de Química, Área de Catálisis, Universidad Autónoma Metropolitana-Unidad Iztapalapa, Av. San Rafael Atlixco No. 186, C.P. 09340, A.P 55-534. México D. F. México.

**ABSTRACT**

The methane dehydrogenation reaction was carried out on Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd catalysts. These were synthesized by wet impregnation of the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd supports at 1 and 10 wt% of neodymium and 1wt% of rhodium using the Nd(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O and RhCl<sub>3</sub>·3H<sub>2</sub>O as precursors.

The reaction was carried out from 400 to 700 °C at intervals of 100 °C with a rate of 5 °C min<sup>-1</sup>. Experiments consisted in a previous thermal treatment to the catalysts with flowing nitrogen for 15 min at room temperature. Then, a pure CH<sub>4</sub> (high purity) feed stream (2 mL min<sup>-1</sup>) was introduced into the reactor, the products were analyzed by gas chromatography. The activity determinations were carried out in a quartz glass microreactor system with a fixed bed at atmospheric pressure and catalyst load of 0.05 g.

The Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, Rh-Nd1% and Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd10% catalysts showed CH<sub>4</sub> conversions of 74, 79 and 75% and selectivities to hydrogen of 89, 65 and 100% respectively at 700 °C. The metal particle size of Rh and the acidity influenced these results; since the catalyst with the largest particle size (Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd10%) ~ 3.4 nm and the lowest acidity, 96  $\mu$ mol g<sup>-1</sup>, was the most selective to hydrogen.

The Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd1% catalysts presented also selectivities towards ethane and ethylene, which came from the mobility of the CH<sub>x</sub> species on Rh surface during the degradation of methane. The performance of the Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Nd10% catalyst is explained by the high interaction of Rh and alumina-Nd. The carbon produced during the reaction was graphitic type which was deposited on the Rh surface and on the support.

The characterization was carried out by X-ray diffraction, N<sub>2</sub> adsorption, TEM, SEM-EDS, pyridine FT-IR and H<sub>2</sub>-TPR. The Rh/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst doped with 10% of neodymium and the particle size of Rh of around 3.4 nm resulted with the best production of hydrogen in the methane dehydrogenation. The graphitic carbon produced during the reaction does not affect significantly the H<sub>2</sub> production, since it is also deposited on the support.

**Keywords:** Hydrogen, Methane decomposition, Rh/Alumina-Nd, TEM

\* Corresponding author: Marina Caballero Diaz, Tel (55)5804-4668 Fax (55)5804-4666  
E-Mail: marcabdi@yahoo.com.mx



**Effect of organic molecule (ethylenediamine) in the preparation of ZnS and ZnS(hybrid) semiconductor in H<sub>2</sub> production**

**C. García Mendoza<sup>a,\*</sup>; S. Ramírez-Rave<sup>a</sup>; J. M. Alvaro<sup>a</sup>; A. A. Flores-Caballero<sup>c</sup>;  
A. Hernández-Gordillo<sup>b</sup>; R. Gómez<sup>a</sup>**

<sup>a</sup> Universidad Autónoma Metropolitana-Iztapalapa, Depto. de Química, Área de Catálisis, Grupo ECOCATAL, Av. San Rafael Atlixco No 186, Mexico 09340, D.F. Mexico.

<sup>b</sup> Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior SN, Ciudad Universitaria, C.P. 04510, Mexico D.F., Coyoacán, Mexico.

<sup>c</sup> Instituto Politécnico Nacional, Barrio la Laguna Ticomán C.P. 07340, México, D.F. México.

**ABSTRACT**

H<sub>2</sub> will become one of the most promising energy sources due to its environmental friendly nature. H<sub>2</sub> generation by heterogeneous photocatalysis from water in the presence of organic molecule as sacrificial electron donor, using semiconductors as photocatalysts, has brought attention in scientist community. ZnS is an adequate semiconductor for the water splitting process since that the position of its conduction band is favorably negative to conduct reduction reaction and it is resistant to the photocorrosion. Diverse research have been focused in the improvement of photophysical properties of ZnS. It has been reported that ZnS modified by organic molecules, increase the photoactivity of the material. In the present work, ZnS and ZnS(hybrid) materials were synthesized by precipitation method. Different ethylenediamine concentrations were used (20, 40, 60 and 80% vol.) in order to prepare the corresponding inorganic and hybrid semiconductor. Photocatalytic H<sub>2</sub> production reaction was carried out in a glass photoreactor with a solution of water/methanol mixture and the corresponding photocatalysts. The hexagonal ZnS and orthorhombic ZnS(hybrid) synthesized materials, have high efficiencies in the production of H<sub>2</sub>. The textural and optical-electronic properties are presented and discussed.

**Keywords:** Photocatalysis, ZnS-Hybrid, Water splitting, Hydrogen production

\* Corresponding author:

Cinthia García Mendoza 52+55 58044669 cinthiagame@hotmail.com

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Emerging electrochemical technologies for hydrogen utilization:  
redox flow batteries**

**I. L. Escalante-García<sup>a\*</sup>; R. F. Savinell<sup>b</sup>; S. M. Durón-Torres<sup>a</sup>**

<sup>a</sup>Unidad Académica de Ciencias Químicas, Universidad Autónoma de Zacatecas, Campus Siglo XXI, Carretera Zacatecas-Guadalajara Km. 6.0, Ejido la Escondida, Zacatecas, México, 98160.

<sup>b</sup>Department of Chemical Engineering, Case Western Reserve University, Cleveland, Ohio, USA.

**ABSTRACT**

Renewable energy sources can supply a significant amount of electrical energy; however, their massive penetration as an alternative energy source has been limited by their variability and intermittent nature. Redox flow battery (RFB) technology has emerged as a very attractive option for energy storage applications that can efficiently maximize the use of renewable energy resources (i.e. wind and solar). Unlike conventional batteries, redox flow battery systems are more attractive for energy storage because they offer more flexible operation, simple electrode reactions, operation at low temperature, longer cycle life, higher overall energy efficiencies and easier scaling-up. The RFB systems have also the important advantage that the energy storage capacity and power density output are independent variables and can be easily modulated. Because of these advantages, the RFB is considered to be one of the most cost-effective energy storage technologies. In the last years, aqueous and non-aqueous RFB chemistries have been explored and investigated as possibilities for practical applications. Current investigations on these RFBs are focused on increasing power density at acceptable efficiencies (70-90%) to allow for a decrease in cell size and, as a consequence, in an overall lower system cost. Recently, novel RFB systems with hydrogen gas and an aqueous electrolyte solution as positive and negative reactants, respectively, have been studied and shown to be a possible high-power and more cost effective system. In this talk, general features and state-of-art of aqueous and non-aqueous RFBs systems are presented. In particular, the fundamental understanding of the key factors limiting the performance of non-aqueous RFB systems in a realistic flow battery design is discussed. Finally, the feasibility of hydrogen as energy source for high-power density RFB, cell design considerations and system costs is also presented. Overall, RFBs seems to be suitable for energy storage applications in conjunction with renewable energy sources, however, several technical limitations still needs to be overcome to obtain more efficient and low-cost systems for faster commercialization.

**Keywords:** Renewable energy, Redox flow batteries, Hydrogen, Energy storage

\* Corresponding author:

Escalante García Ismailia L., Tel: +524929256690 Ext. 4655; e-mail: ismailiae@gmail.com



**Hydrogen adsorption process in Magnesium-Aluminum compounds  
(Mg<sub>25</sub>Al, Mg<sub>50</sub>Al and MgOAl) varying pressure and temperature  
conditions**

**J. L. Iturbe – García<sup>a,\*</sup>; B. E. López – Muñoz<sup>a</sup>**

<sup>a</sup>Departamento de Química, Instituto Nacional de Investigaciones Nucleares, Km 36.5 Carretera México-Toluca s/n, la Marquesa, C.P. 52045, Ocoyoacac, Estado de México, Tel: (01-55) 53297200 ext. 12274, fax: (01-55) 53297301

**ABSTRACT**

In this work the H<sub>2</sub> adsorption/desorption process in various magnesium – aluminum compounds is presented. These Mg and Al compounds were submitted to hydrogenation process in both Thermogravimetric Analyzer and a micro reactor systems. In the last equipment, pressure, temperature and contact time were varied trying to perform hydrogenation experiments in the best environmental conditions particularly temperature and pressure parameters. The Mg<sub>50</sub>Al, Mg<sub>25</sub>Al alloys were used in this investigation, for decreasing its particle size high energy mechanical milling was performed by placing 2 g of each sample (Mg<sub>50</sub>Al and Mg<sub>25</sub>Al) and milling media into a stainless steel vial for milling during only a period of 5 hr using white gasoline as process control agent and without control agent for Mg<sub>50</sub>Al and Mg<sub>25</sub>Al respectively. Magnesium oxide-aluminum (MgOAl) phase was also used for hydrogen adsorption, this material was prepared in an electric tube furnace under normal atmosphere from intermetallics described above. The hydrogenation process was carried out by placing the samples into the micro reactor under vacuum for one hour at 300° C, then the system was cooled to 50° C, immediately hydrogen was put in contact with the materials at a pressure of 20 atm for 5 min. The samples were analyzed before and after hydrogenation process by TGA, SEM, XRD and gas chromatography. The results indicate that these materials adsorb hydrogen at moderate pressure and temperature conditions. The hydrogen concentration values of each compound are reported in weight percentages. The technique of gas chromatography was used to verify the presence of hydrogen in the compounds studied according to the results obtained by the TGA system.

**Keywords:**Hydrogen adsorption, Magnesium-aluminum compounds, Thermogravimetric analysis, Gas chromatography

\* Corresponding author:

J. L. Iturbe – García

Tel: (01-55) 53297200 ext. 12274, fax: (01-55) 53297301, C.P. 52045; mail: joseluis.iturbe@inin.gob.mx

## **Flow of hydrogen adapted to cell fuels using recycled aluminum**

**J.E. Salas-Weber; M. Abatal; I. E. Castro; J. M. Sierra; S. Martínez-Vargas;**  
**V. Rodríguez-Iglesias; C. Patiño-Carachure\***

Facultad de Ingeniería, Universidad Autónoma del Carmen, Campus III, Fracc. Mundo Maya, C.P. 24115, Cd. del Carmen, Cam., Mex.

### **ABSTRACT**

Fuel cells convert chemical energy into electrical energy without combustion. Hydrogen based fuel cells are promising systems for future hydrogen propelled vehicles, stationary and mobile applications. The problems about the technology of cell fuels are storage and production of  $H_2$ . Thus, in this investigation different morphologies of recycled aluminum such as powders, ingots and rings were used to produce a  $H_2$  flow sufficient for be assisted to a fuel cell. Different concentrations of NaOH, KOH (0.25, 0.75, 1.25 mol/L) were employed into solution of 100 ml distilled water. The result indicate, that during 120 minutes the production of hydrogen is already 4 to 9 ml/min for ring at 1.25 mol/L NaOH). The hydrogen generation is faster to powders, during 10 minutes it reach from 20 to 100 mL/min. These results can be applied to produce  $H_2$  sufficient for feeding fuel cells.

**Keywords:** Recycled aluminum, Hydrogen generation, NaOH, KOH

\* Corresponding author:

Cristobal Patiño Carachure, Phone: +52(938)3811018-ext.1702, Email: cpatino@pampano.unacar.mx

**Synthesis, characterization and photocatalytic evaluation of**  
 **$M_{1-x}M'_xWO_4$  ( $M, M' = Ni, Co, Cu$  and  $Mn$ ) tungstates**

**X. A. López<sup>1,2</sup>; A. F. Fuentes<sup>2</sup>; M. Meléndez Zaragoza<sup>3</sup>;  
J. A. Díaz Guillén<sup>1</sup>; A. Lopez Ortiz<sup>3</sup>; V. Collins-Martínez<sup>3\*</sup>**

<sup>1</sup>Instituto Tecnológico de Saltillo, Blvd. V. Carranza No. 2400, Col. Tecnológico Saltillo, C. P. 25280 Coahuila, México

<sup>2</sup>CINVESTAV del IPN, Unidad Saltillo, C.P. 25900, Ramos Arizpe, Coahuila México

<sup>3</sup>Centro de Investigación en Materiales Avanzados S. C., Miguel de Cervantes 120, C. P. 31136, Chihuahua, Chih. México

**ABSTRACT**

Photocatalysis is a technology that can be applied to solve environmental and energy problems such as the production of  $H_2$  from the dissociation of the water molecule. Tungstates exhibit many potential applications in different areas of technology due to their excellent electrical properties. Nanostructured tungstate materials are known for their wide applications in conventional catalysis, as scintillator material, in photoluminescence, optical fibres and as materials in microwave technology. Even though these present enough chemical and thermal stability, very scarce reports are found in the literature related to their uses as photocatalysts for hydrogen production through water splitting. The aim of the present study is the synthesis and characterization of family tungstate  $MWO_4$  ( $M = Co, Cu, Mn$  and  $Ni$ ) materials through co-precipitation in order to evaluate their photocatalytic activity towards the production of  $H_2$  within the visible light range. Characterization was performed by XRD, BET, UV-Vis and SEM, while the photocatalytic evaluation was as follows: 200 mg of  $CuWO_4$ ,  $CoWO_4$ ,  $MnWO_4$  and  $NiWO_4$  powders were individually suspended in water and methanol, the latter used as a sacrificial agent. The water suspension was placed inside a sealed quartz batch photoreactor under constant stirring and illuminated by a 250W mercury lamp for 8 h with gas evolution being monitored by gas chromatography (GC). Preliminary results indicate that the employed synthesis method was effective to obtain the required crystalline phase. However, optimal conditions are needed to decrease particle size and increase the tungstate surface areas. The bandgap energy of these tungstates was found to be within the visible light spectrum with a variation between 2.24 eV for  $CoWO_4$  to 2.56 eV for  $MnWO_4$ , respectively. Maximum  $H_2$  production was achieved by sample  $MnWO_4$  with  $139 \mu\text{mH}_2/\text{g}_{\text{cat}}$ , while the lowest production was observed for sample  $CoWO_4$  with  $24 \mu\text{mH}_2/\text{g}_{\text{cat}}$ . From these preliminary results it can be inferred that simple and mixed metal transition tungstates can be considered as potential candidates, as photocatalysts for  $H_2$  production via the splitting of the water molecule under visible light irradiation.

**Keywords:**  $H_2$  generation, Water splitting, Photocatalysis, Tungstates

\* Corresponding author: Virginia Collins Martinez, phone: +526144391129; e-mail: virginia.collins@cimav.edu.mx





## **Direct oxidation fuel cells**

**Synthesis, characterization and evaluation of Ni@Pt and Fe@Pt nanoparticles with core-shell structure to the electro-oxidation reaction of ethanol**

**A. Gómez-Monsiváis<sup>a</sup>; J. Maya-Cornejo<sup>b</sup>; J. Ledesma-García<sup>c</sup>; M. Guerra-Balcázar<sup>c</sup>;  
N. Arjona<sup>d\*</sup>**

<sup>a</sup>Tecnológico Nacional de México, Instituto Tecnológico de Tijuana, Tijuana, B. C., C.P. 22414, México.

<sup>b</sup>Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Pedro Escobedo, Qro., C.P. 76703, Mexico.

<sup>c</sup>Facultad de Ingeniería, División de Investigación y Posgrado, Universidad Autónoma de Querétaro, Centro Universitario Cerro de las Campanas, Querétaro, Qro., C.P. 76010, México.

<sup>d\*</sup> Centro de Investigación y Desarrollo Tecnológico en Electroquímica S.C. Subsede Tijuana. Tijuana, B.C., C.P. 22444, México.

**ABSTRACT**

The ethanol electro-oxidation reaction is interesting because of ethanol has low toxicity and higher theoretical energy density compared to methanol. Pt is -by excellence- the best electrocatalyst for this reaction. However, it has an elevated cost which makes it impractical for its commercial use. One strategy to overcome this issue is by employing Pt-M (M = transition metal) bimetallic mixtures in order to reduce both the amount of Pt and the poisoning effect of Pt by adsorption of carbon monoxide (CO). In this work, Fe@Pt and Ni@Pt nanoparticles were synthesized through an aqueous chemical reduction method, using polyvinylpyrrolidone (PVP) as a surfactant, L-ascorbic acid as reducing agent and sodium bromide (NaBr) as an additive. These materials were characterized by physicochemical techniques (XRD, XRF, TGA and TEM). In addition, they were electrochemically characterized by cyclic voltammetry (CV) in alkaline medium. The physicochemical characterization revealed the presence of small sizes NPs (in the order of 5 to 12 nanometers). The metal mass composition of electrocatalysts was determined by XRF, where Fe@Pt exhibited a composition of Fe<sub>30</sub>Pt<sub>70</sub>, and Ni@Pt of Ni<sub>70</sub>Pt<sub>30</sub>. Electrochemical profiles showed only the typical response of Pt-based materials in alkaline media. On the other hand, both electrocatalysts showed the highest activity at 1M ethanol exhibiting oxidation potentials of -0.226 and -0.253 V vs. NHE for Fe@Pt and Ni@Pt, respectively. At this concentration, maximum current densities of 53.42 and 62.91 mA cm<sup>-2</sup> were achieved for Fe@Pt and Ni@Pt, respectively. Through these results, it is concluded that Ni@Pt showed better activity in terms of both, potential and current density than Fe@Pt nanoparticles using lower amount of Pt.

**Keywords:** Electrocatalysis, Fuel cells, Ethanol oxidation, Nanotechnology

\* Corresponding author: N. Arjona, Tel. +52 (664) 645 32 78, C.P. 22444, E-mail: wvelazquez@cideteq.mx



**Pd and Pd-NiO as anodes in a paper-based ethanol membraneless nanofluidic fuel cell**

**C. López-Rico<sup>a,d</sup>; J. Galindo-de-la-Rosa<sup>b</sup>; E. Ortiz-Ortega<sup>b</sup>; J. Ledesma-García<sup>b</sup>;  
M. Guerra-Balcázar<sup>b</sup>; L. G. Arriaga<sup>c</sup>; N. Arjona<sup>d\*</sup>**

<sup>a</sup>Instituto Tecnológico de Tijuana, Tijuana, B. C., C.P. 22414, México.

<sup>b</sup>Facultad de Ingeniería, División de Investigación y Posgrado, Universidad Autónoma de Querétaro, Centro Universitario Cerro de las Campanas, Querétaro, Qro., C.P. 76010, México.

<sup>c</sup>Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Pedro Escobedo, Qro., C.P. 76703, México.

<sup>d</sup>Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Unidad Tijuana, Tijuana, B.C., C.P. 22444, México.

**ABSTRACT**

Pd and Pd-NiO nanoparticles were synthesized using a protic ionic liquid (2-hydroxy ethylammonium formate) as a green method. According with TEM micrographs, nanoparticle sizes of 20 and 8.1 nm were obtained for Pd and Pd-NiO, respectively. Thermogravimetric analyzes exhibited metal mass content of 25.89% for Pd/C (Vulcan carbon) and 5.99% for Pd-NiO/C. Both electrocatalysts showed activity toward ethanol electro-oxidation (tested at 0.5, 1, 2 and 3 M). Furthermore, Pd-NiO/C exhibited higher current density than Pd/C (i.e. 20-fold at 3 M ethanol). A paper-based membraneless nanofluidic fuel cell was constructed using a paper plotter. The electrodes were made of carbon nanofoam and placed altogether with a polymeric pattern as separator (Silastic) between the paper sheets. In this cell design, streams flow through electrodes to utilize the high surface area of carbon nanofoam (450 m<sup>2</sup>/g). Ethanol at several concentrations was used as fuel; meanwhile, an oxygen-saturated solution combined with oxygen from air was used as oxidant. At 0.5 M ethanol, a maximum cell voltage of 0.66 V was achieved. Also, a current density of 100 mA/cm<sup>2</sup> and a power density of 17.65 mW/cm<sup>2</sup> were obtained.

**Keywords:** Membraneless, Fuel cell, Ethanol, Microfluidic, Electrocatalysis

\*Corresponding author

**Development of Nickel hollow spheres electrocatalysts for ethanol  
electrooxidation in alkaline media**

**A. Altamirano-Gutiérrez<sup>a</sup>; G.E. Martínez-Tapia<sup>a</sup>; L.C. Ordóñez<sup>a,\*</sup>**

<sup>a</sup>Centro de Investigación Científica de Yucatán, A.C., Parque Científico Tecnológico de Yucatán, Carretera Sierra Papacal – Chuburná Puerto, km 5. Sierra Papacal, Mérida, Yucatán, C.P. 97302.

**ABSTRACT**

We report the synthesis of nickel hollow spheres and its structural, morphological and electrochemical catalytic evaluation for ethanol oxidation reaction in 1.0 M NaOH. Materials were prepared by the microemulsion method from  $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ , NaOH and using  $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$  as reducing agent. Dodecyl sodium sulfate (SDS) was used as soft template. The concentration of each component was carefully controlled up to forming colloidal  $\text{Ni}(\text{OH})_2$  particles which, were reduced to obtain the nickel spheres. The synthesized materials were characterized by X-Ray diffraction (XRD), scanning electron microscope (SEM). The surface morphology was analyzed by atomic force microscope (AFM). Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques were performed in order to evaluate the catalytic activity for the ethanol oxidation reaction in alkaline medium. The synthesized material with microemulsion conditions of 96%  $\text{H}_2\text{O}$ -3% SDS -1% pentanol presented the highest current density for ethanol oxidation peak:  $147 \text{ mAcm}^{-2}$  at 0.722 V. Results indicate that metallic Ni microspheres with diameters between 0.2 and 1.4 micrometers are potential candidates for its use as anodes in alkaline direct alcohol fuel cells (A-DAFCs).

**Keywords:** Nickel hollow microspheres, Microemulsion, Ethanol electrooxidation, Alkaline direct alcohol fuel cells

\* Corresponding author:  
Luis Carlos Ordóñez López  
Email: lcol@cicy.mx

## **Methanol Oxidation on Au@Pt and Cu@Pt Core-Shell Electrocatalysts**

**N. Chávez-Pineda<sup>a</sup>; G. Vázquez-Huerta<sup>a,\*</sup>; S. Corona-Avedaño<sup>a</sup>**

<sup>a</sup>Materials Department, Universidad Autónoma Metropolitana, Av. San Pablo 180, Reynosa Tamaulipas, C.P. 02200, México D.F., México.

### **ABSTRACT**

In this work, the methanol oxidation on core-shell Au@Pt and Cu@Pt electrocatalysts is studied. For this purpose, the core-shell nanoparticlessupported on carbon Vulcan XC-72R were prepared by using a two-step colloidal method. The electrochemical behavior of Au@Pt/C and Cu@Pt/C was evaluated by using anodic stripping voltammetry, cyclic voltammetry and chronoamperometry ( in a three-electrode electrochemical cell and 0.5M H<sub>2</sub>SO<sub>4</sub> + 1M methanol as working solution). The physical characterization by scanning-transmission electron microscopy (STEM) showed that the synthesis procedure generates quasi-spherical nanoparticles of ~22nm for Au@Pt and 12 nm for Cu@Pt/C. X-ray diffraction (XRD) results showed that in both cases, Au@Pt and Cu@Pt, the crystallographic structure of the core is maintained, inferring that an Pt epitaxial growth is produced. The electrochemically active surface area (ECSA) was evaluated in all casesby using anodic stripping voltammetry; the values of ECSA were used to normalize the currents obtained during methanol oxidation experiments. From cyclic voltammetry results it was found that Au@Pt/C catalyst presented the highest values of current density for methanol oxidation, also the peak potentials ( $E_{p,1}$  and  $E_{p,2}$ ) of methanol oxidation are less positive than those showed on Cu@Pt/C which indicates that a smaller activation energy is needed on Au@Pt/C for methanol oxidation to occur. Similar results were obtained from chronoamperometric experiments; the steady-state current density ( $i_{ss}$ ) of methanol oxidation is higher when Au@Pt/C catalyst is used. For comparison purposes, Pt/C was also prepared, and in chronoamperometric experiments the current density obtained for methanol oxidation,at initial times, was higher on Pt/C than on the other catalysts; however after 1200 s, it diminishes below the  $i_{ss}$  value showed by Au@Pt/C, this behavior could be related to the poisoning effect of CO on Pt, the poisoning effect is diminished on Au@Pt/C electrocatalyst.

**Keywords:** Methanol oxidation, Core-shell nanoparticles, Gold-platinum, Copper-platinum

\* Corresponding author:

G. Vázquez-Huerta, 52 (55) 53189356, gvh@correo.azc.uam.mx

## **Formic Oxidation on Core-Shell Au@Pt<sub>x</sub>/C Electrocatalyst**

**L. U. Martínez-Fernández<sup>a</sup>; G. Vázquez-Huerta<sup>a,\*</sup>; S. Corona-Avedaño<sup>a</sup>**

<sup>a</sup>Materials Department, Universidad Autónoma Metropolitana, Av. San Pablo 180, Reynosa Tamaulipas, C.P. 02200, México D.F., México.

### **ABSTRACT**

Pt is the best up-to-date known catalyst; however platinum can be easily poisoned with CO which is produced during formic acid oxidation. To solve this problem, core-shell nanocatalysts (Au@Pt<sub>x</sub>) with variable Pt-thickness are synthesized by using a two-step colloidal method, the synthesized catalysts were prepared using the following Au:Pt proportions: 2:1, 1:1, 1:2 and 1:4. The electrochemical behavior of Au@Pt catalysts supported on carbon Vulcan XC-72R (denominated Au@Pt<sub>x</sub>/C) was evaluated with electrochemical techniques in a three-electrode electrochemical cell and 0.5M H<sub>2</sub>SO<sub>4</sub> + 0.5M HCOOH as working solution. The physical characterization of Au@Pt<sub>x</sub>/C catalysts was carried out by scanning-transmission electron microscopy (STEM) and X-ray diffraction (XRD). Electrochemical results from *I* vs *E* curves showed that 2:1 Au@Pt/C electrocatalyst produced the highest current density in comparison with 1:1, 1:2 and 1:4 Au@Pt<sub>x</sub>/C catalysts. The electrochemically active surface area (ECSA) was evaluated in all cases by using anodic stripping voltammetry; the values of ECSA were used to normalize the currents obtained during the formic acid oxidation experiments. The physical characterization by scanning-transmission electron microscopy (STEM) showed that the synthesis procedure generates quasi-spherical nanoparticles of 18nm, 16 nm, 18nm y 21 nm for 2:1, 1:1, 1:2 and 1:4 Au@Pt<sub>x</sub>/C catalysts. XRD results showed that in all cases the crystallographic structure of gold-core is maintained inferring that an epitaxial growth of Pt on Au is produced.

**Keywords:** Formic acid oxidation, Gold-platinum, Core-shell catalysts

\* Corresponding author:

G. Vázquez-Huerta, 52 (55) 53189356, gyh@correo.azc.uam.mx



## **High performance Pd-based catalysts for electro-oxidation of formic acid**

**P.C. Meléndez-González<sup>a</sup>; F.J. Rodríguez-Varela<sup>a,b,\*</sup>; D. Morales-Acosta<sup>c</sup>**

<sup>a</sup> Programa de Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, 25900, México.

<sup>b</sup> Programa de Nanociencias y Nanotecnología, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, 25900, México.

<sup>c</sup> Centro de Investigación en Química Aplicada, Depto. Procesos de Transformación, Blvd. Enrique Reyna Hermosillo 140, Saltillo, Coahuila, 25294, México.

### **ABSTRACT**

In this study, 20 % Pd-M/C (where M= Au, Fe<sub>3</sub>O<sub>4</sub>, CeO<sub>2</sub>) nanocatalysts with an Pd:M atomic ratio of 1:1 were synthesized by the impregnation-reduction method. Their catalytic activity for the formic acid oxidation reaction (FAOR) was evaluated in 0.5 M H<sub>2</sub>SO<sub>4</sub>. The results have been compared with those of a Pd/C catalyst prepared by the same procedure. EDS analysis of the anodes indicated a chemical composition similar to the nominally expected. XRD results showed nanosized catalysts having crystalline structure, with an average crystallite size between 3.5 and 5.5 nm. The evaluation of performance for the FAOR indicated that the three bimetallic catalysts have higher catalytic activity than Pd/C. Among them, the novel Pd-Fe<sub>3</sub>O<sub>4</sub>/C showed the higher catalytic activity. The peak maximum current density (in mA mg<sub>Pd</sub><sup>-1</sup>) recorded for Pd-Fe<sub>3</sub>O<sub>4</sub>/C was 285.05, which is higher than that of Pd-Au/C 120.64 and Pd-CeO<sub>2</sub>/C 87.71, and significantly more intense than Pd/C (22.15). Besides, the on-set potential of the FAOR recorded for Pd-Fe<sub>3</sub>O<sub>4</sub>/C (0.20 V) and Pd-CeO<sub>2</sub>/C (0.23 V) were slightly lower than Pd-alone (0.24 V). It has been concluded that the use of inexpensive co-catalysts such as Fe<sub>3</sub>O<sub>4</sub> (and CeO<sub>2</sub> to some extent) had a synergistic effect on Pd, which helped to improve the performance for the FAOR. With this approach, the amount of Pd in the electrodes was reduced, having as a result low-cost anodes for Direct Formic Acid Fuel Cells.

**Keywords:** Formic acid oxidation reaction, Low-cost Fe<sub>3</sub>O<sub>4</sub> co-catalyst, Direct formic acid fuel cells

\* Corresponding author:

F.J. Rodríguez Varela, 52 +844 438-9600 (Ext. 8526), 25900, javier.varela@cinvestav.edu.mx

**Development of a direct methanol fuel cell with polymer electrolyte membrane**

**J. Montalvo<sup>a</sup>, B. Escobar<sup>b</sup>, R. Barbosa<sup>c</sup>, G. Rodriguez-May<sup>a</sup> Victor M. Sanchez<sup>c</sup>,  
J.C. Cruz<sup>a\*</sup>**

<sup>a</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 70013, México

<sup>b</sup>Centro de Investigación científica de Yucatán, A.C., Calle 43 No. 130 Colonia Chuburná de Hidalgo, Mérida, Yucatán 97200, México

<sup>c</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Quintana Roo 77019, México

**ABSTRACT**

The Direct methanol fuel cell (DMFC) is considered as a highly promising power source. It is based on polymer electrolyte membrane fuel cell (PEMFC). The conceptually promising features of a direct methanol fuel cell have stimulated vigorous research efforts on the electrooxidation of methanol in acid media. Many different electrode materials have been tested for their activity toward the anodic oxidation of methanol, including single-crystal surfaces to gain a more fundamental understanding of methanol electrocatalyst. It possesses a number of advantages such as a liquid fuel, quick refueling, low cost of methanol and the compact cell, design making it suitable for various potential applications including stationary and portable applications. This work studied the design, fabrication of a Direct Methanol Fuel Cell. The structure of the direct methanol fuel cell (DMFC) consisted of two electrocatalytic electrodes; PtPd/C catalyst cathode and Pt/C catalyst anode. The material was deposited by hot spray technique, the PtPd/C (30:70 wt%) catalyst loading was  $1 \text{ mg cm}^{-2}$  and Pt/C (30% wt, Pt) as hydrogen electrode. The electrochemical parameters were determined using the techniques of linear voltammetry, electrochemical impedance spectroscopy, chronoamperometry and chronopotentiometry. It was determined the amount at 25°C. A Direct methanol fuel cell for science in schools and higher secondary education was obtained.

**Keywords:** Methanol, PtPd/C, DMFC

\* Corresponding author:

Dr. Julio Cesar Cruz Argüello, +983 1043002, México [jrcruz@itchetumal.edu.mx](mailto:jrcruz@itchetumal.edu.mx)

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Innovative functionalization of graphene to increase the catalytic activity of Pt/Gr electrocatalyst for the Methanol Oxidation Reaction (MOR)**

**A.A.Siller-Ceniceros<sup>a</sup>; M. E. Sánchez-Castro<sup>a,b</sup>; D. Morales-Acosta<sup>c</sup>;  
E. Martínez-Guerra<sup>d</sup>; F.J. Rodríguez-Varela<sup>a,b\*</sup>**

<sup>a</sup>Programa de Nanociencias y Nanotecnología, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coah., C.P. 25900, México.

<sup>b</sup>Grupo de Sustentabilidad de los Recursos Naturales, Cinvestav Unidad Saltillo, Av. Industrial Metalúrgica No. 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coah., México, 25900

<sup>c</sup>Centro de Investigación en Química aplicada, Blvd. Enrique Reyna No. 140, San José de los Cerritos, Saltillo, Coah. C.P. 25294, México.

<sup>d</sup>Centro de Investigación en Materiales Avanzados, S.C. Alianza Norte 202, PIIT, Carretera Monterrey-Aeropuerto Km. 10, Apodaca NL 66600, México.

**ABSTRACT**

The aim of this work was to functionalize partially reduced graphene (Gr), with two different ruthenium compounds: 1)  $\text{RuCl}_3 \cdot \text{XH}_2\text{O}$  (Rucom) and 2)  $[(\eta^6\text{-C}_6\text{H}_5\text{OCH}_2\text{CH}_2\text{OH})\text{RuCl}_2]_2$  an organometallic ruthenium (II) arene compound (Ru-dim) by the Schlenk technique. EDS characterization of Gr confirmed the presence of 21.47 and 6.62 (wt. %) Ru when functionalization was carried out with Ru-dim and Ru-com respectively. With these functionalized and non-functionalized Gr, Pt/Gr nanoelectrocatalysts were synthesized with the polyol technique. EDS analysis revealed Ru content of 11.70 and 6.54 (wt. %), and Pt of 13.90 and 18.09 (% wt.) at Pt/Gr<sub>Ru-dim</sub> and Pt/Gr<sub>Ru-com</sub>, respectively. The Pt content of Pt/Gr (non-functionalized Gr) was 20.51 (wt. %). During the evaluation of catalytic activity for the MOR in acid media containing 0.5 M MetOH, Pt/Gr<sub>Ru-dim</sub> reached a current density of  $45.07 \text{ mA cm}^{-2}$ , greater than 31.15 and  $11.31 \text{ mA cm}^{-2}$  generated by Pt/Gr<sub>Ru-dim</sub> and Pt/Gr, respectively. Furthermore, the on-set potential at Pt/Gr<sub>Ru-dim</sub> was 262.97 mV, significantly more negative than the potentials at Pt/Gr<sub>Ru-com</sub> and Pt/Gr (380.49 and 402.04 mV). The results showed that the functionalization of Gr with Rudim increased remarkably the catalytic activity for the MOR, suggesting a possible Pt-Ru metal-metal interaction that promotes the anodic reaction.

**Keywords:** Graphene, Organometallic compounds, Functionalization and nanoelectrocatalyst

\* Corresponding author:

F.J. Rodríguez-Varela, 01-52-(844)438-9600 ext. 8526,  
javier.varela@cinvestav.edu.mx



**Synthesis and characterization of Sn@Pt/C and Ru@Pt/C core-shell nanocatalysts for the EOR**

**D. González-Quijano<sup>a</sup>; W.J. Pech-Rodríguez<sup>a</sup>; J.I. Escalante-García<sup>a,b</sup>;  
G. Vargas-Gutiérrez<sup>a,b</sup>; F.J. Rodríguez-Varela<sup>b,c,\*</sup>**

<sup>a</sup>Ingeniería Metalúrgica e Ingeniería Cerámica

<sup>b</sup>Sustentabilidad de los Recursos Naturales y Energía

<sup>c</sup>Programa de Nanociencias y Nanotecnología

Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe.  
Ramos Arizpe, Coahuila, C.P. 25900, México.

**ABSTRACT**

Pt-alone anodes have shown low performance for the complex oxidation of alcohols to CO<sub>2</sub>. It involves the breaking of C-C bonds during their dissociative adsorption producing intermediates (i.e. CO-like species) that strongly adsorb on Pt active sites, depolarizing it. Core-shell nanostructures have shown high catalytic activity for the oxidation of alcohols. In this work, M@Pt/C core-shell catalysts (where M: Sn and Ru) with nominal Pt:Matomic ratio of 1:1 were synthesized by a polyol reduction process in two successive steps. The Metal:Vulcan support ratio was 20:80 (wt. %). The electrocatalytic activity of the catalysts was studied in acid media for the Ethanol Oxidation Reaction (EOR). XRD characterization of Sn@Pt/C and Ru@Pt/C shows the typical peaks of carbon and fccPt. The particle size calculated with the Scherrer equation was 2.47 and 1.96 nm for Sn@Pt/C and Ru@Pt/C, respectively. Chemical analysis by EDS indicated that the atomic ratio was higher than the expected: 2.4:1 in the case of Sn@Pt and 2.5:1 for Ru@Pt. The CO stripping experiments indicated that the core-shell catalysts adsorb the CO at lower potentials than Pt/C. The EOR characterizations showed that the reaction started at lower onset potentials (404 mV) in the case of Sn@Pt/C, with a maximum peak current density of 313.40 mA mg<sub>Pt</sub><sup>-1</sup>. The values for Ru@Pt/C were 322 mV and 266.71 mA mg<sub>Pt</sub><sup>-1</sup>, while those of Pt/C were 450 mV and 427.57 mA mg<sub>Pt</sub><sup>-1</sup>. After accelerated degradation test, the core-shell catalysts did not show Electrochemically Active Surface Area losses, demonstrating their high stability. Furthermore, the chronoamperometry measurements showed that the catalysts have a similar behavior than Pt/C. These results demonstrated that the core-shell catalysts have better performance and stability during the EOR than the Pt/C catalyst.

**Keywords:** Core-Shell catalysts, Sn@Pt and Ru@Pt, EOR, Direct alcohol fuel cells

\* Corresponding author:

F.J. Rodríguez-Varela, Phone number: +52(844)438-9600 ext. 8526, E-mail: javier.varela@cinvestav.edu.mx



**Micro-direct methanol fuel cells**

**P. Mendoza-Correa<sup>a</sup>; V. Galvan<sup>b</sup>; K. Domalon<sup>b</sup>; S. Sotez<sup>b</sup>; F. Gomez<sup>b</sup>; M. Hinojosa<sup>a</sup>**

<sup>a</sup>Facultad de Ingeniería Mecánica y Eléctrica, Universidad Autónoma de Nuevo León, Pedro de Alba S/N, Ciudad Universitaria, 66450 San Nicolás de Los Garza, NL, Mexico.

<sup>b</sup>California State University, Los Angeles, 5151 State University Drive, Los Angeles, CA, 90032-8202.

**ABSTRACT**

The development of advanced technologies to generate alternative energy sources at low cost, which does not require the use of fossil fuels and can be used in small portable devices, has significantly increased. For example, fuel cells are simple to operate, have high energy conversion and cause no harm to the environment. One of the newest developments in this field is the microfluidic fuel cells (MFCs). The MFC paper-based works in a standard lateral flow test format, the porosity of the material allows separating the fuel and oxidant species throughout two parallel streams without an ionic exchange membrane or external pumps.

This work describes its fabrication using a paper microfluidic platform. The fuel cells use formate as the anode fuel and hydrogen peroxide as cathode oxidant. By using these materials has been achieved a maximum power density of nearly  $1.2 \text{ mW mg}^{-1} \text{ Pd}$ . The MFC achieves a current density of  $3.5 \text{ mA cm}^{-3}$ . It is also demonstrated that the MFC does not require continuous flow of fuel and oxidant to produce power.

**Keywords:** Fuel cells, Microfluidics, Membraneless, Laminar flow

\* Paola Alejandra Mendoza Correa  
(044) 811 216 8955  
paolaamendoza@gmail.com

## **Fuel cells components and stacks**



## **Optimization of stack performance of low power PEM fuel cells**

**R. Moreno-Flores<sup>a</sup>; E. Escobedo<sup>\*a</sup>; D. Pacheco<sup>a</sup>; M. Smit<sup>a</sup>**

<sup>a</sup>Unidad de Energía Renovable, Centro de Investigación Científica de Yucatán. Calle 43#130 Col. Chuburna de Hidalgo, CP. 97200, Mérida Yucatán, México.

### **ABSTRACT**

For a PEMFC under operation, different causes of performance loss exist. Performance loss can increase when the system is scaled up to higher power. In this work the performance of low-power stacks manufactured in CICY is optimized through studies of the behavior and performance of single cells and stacks of own fabrication, and results are compared to commercial cells. Several electrochemical techniques are used, such as: polarization curves, electrochemical impedance spectroscopy, cyclic voltammetry. These provide insight into the performance of the cell and stack in operation, as well as into the different causes of losses, such as electrical resistance and fuel crossover. In addition to these techniques, SEM is used to evaluate the morphology and uniformity of the catalytic layer. In the first stage of work scaling and operating conditions of the single cell were analyzed in detail, the second stage focused on the manufacturing process, the design and materials of the components of the stack were established. The results demonstrate that for cells with catalyst layers deposited by electrospray the maximum power density of the single FC is higher than for cells prepared with the technique of dropping. The increase is significant, from 208 to 270 mW/cm<sup>2</sup>. Also, the optimization of the hot-pressing process of the MEA resulted in an improvement of the maximum power density up to 310 mW/cm<sup>2</sup>, while minimizing the canal-rib ratio improved the FC performance with about 16%. Compared to commercial PEMFC's, the performance however, is still low, which is likely related to the type of materials used.

**Keywords:** Proton exchange membrane fuel cell, Stack, Electrochemical techniques

\* Corresponding author:

E. Escobedo, Unidad de Energía Renovable, Centro de Investigación Científica de Yucatán. Calle 43#130 Col. Chuburna de Hidalgo, CP. 97200, Mérida Yucatán, México.

**Performance of a microtubular SOFC with an LSCF based composite as cathode**

**C. I. Ramos-Villegas; H. J. Ávila-Paredes\***

Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana, Unidad Iztapalapa, Av. San Rafael Atlixco 186, Col. Vicentina, C.P. 09340, D.F, México.

**ABSTRACT**

Solid Oxide Fuel Cells (SOFC's) are electrochemical devices for converting chemical energy into electrical energy with efficiencies close to 60%. Conventional SOFC's operate at temperatures near 1000 °C; the material generally used as an electrolyte is yttria-stabilized zirconia (YSZ). However, under these conditions there are some drawbacks like components degradation and the restriction of the type of materials to be used for interconnectors and supports, which increases the cost of these devices. Hence, there is a current trend in terms of research to build SOFC's operating at intermediate temperatures (500-700 °C). At this temperature range, gadolinium doped ceria (GDC), is a viable material to be used as electrolyte because of its high ionic conductivity in the 500-700 °C range. Traditionally, SOFC's applications are in stationary power generation systems, however microtubular SOFC's have recently attracted much attention due to its lower operating temperature, higher tolerance to thermal cycles, faster start-up capacity and higher volumetric power densities compared to conventional tubular SOFC's. The present study is centered on the analysis of the performance of a microtubular SOFC. The prototype was fabricated based on a dip coating technique on a sacrificial core; a cermet of  $\text{Ni-Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-x}$  was used as the anode,  $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-x}$  as the electrolyte, and  $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-x}$ - $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$  as the cathode. Electrical measurements of the cell were performed by voltammetry; the cell performance was evaluated based on the polarization curves at 500, 550 and 600 °C.

**Keywords:** Solid oxide fuel cell, Cerium oxide, LSCF, Dip coating

\* Corresponding author:

H. J. Ávila Paredes, (52) 55 58 04 46 00 (ext. 2252), [hjap@xanum.uam.mx](mailto:hjap@xanum.uam.mx)

**Effect of surfactant concentration and metal salt molar ratio on the stability, structure and activity in ORR of Ni@Pt-Pd core-shell**

**C. E. García-Sánchez<sup>a,\*</sup>; J. F. Pérez-Robles<sup>a</sup>; I. E. Pech-Pech<sup>a</sup>**

<sup>a</sup>Dept. of Materials, CINVESTAV-IPN, Libramiento Norponiente 2000, Fracc. Real de Juriquilla, C. P. 76230 Querétaro, Qro., México

**ABSTRACT**

During last years different materials have been produced and tested looking for a reduction in the use of noble metals in the cathode catalyst of polymer electrolyte fuel cells (PEMFCs) for the oxygen reduction reaction (ORR). Core-shell materials are a promising alternative to reach this goal. Due to their structure a non-noble metal can be used as core while shell can be composed of a thin layer of pure or alloyed noble metals. However incorporation of non-noble metals must be performed carefully because the acid environment within a PEMFC could corrode core if not appropriately covered by shell. In this work a core-shell material with nickel as core and a platinum-palladium alloy as shell was synthesized by chemical reduction of metal salts using NaBH<sub>4</sub> in aqueous media. The particles thus produced were then supported on carbon black (Vulcan XC-72). The effects of surfactant concentration (sodium citrate) and molar ratio of metal salts on structural and electrochemical properties in acid media were studied. The obtained materials were characterized through X-ray Diffraction and Dynamic Light Scattering (for particle size measurement). Cyclic Voltammetry and Linear Voltammetry were also performed to evaluate their stability and catalytic activity in ORR respectively. X-ray Diffraction and Cyclic Voltammetry results suggest the actual formation of core-shell structures because only Pt-Pd alloy properties were displayed. Linear Voltammetry also proved this particles were active in ORR. Results allow a better understanding of relationship among studied synthesis variables, structural properties, stability and activity in ORR. Besides this information contributes in finding an optimum cathode catalyst of low cost for application in a PEMFC and could be of help if it is desired to tune this core-shell to match any other specific application.

**Keywords:** Core-shell, ORR activity, Non-noble metal, Synthesis variables effect

\* Corresponding author:

C. E. García-Sánchez, Tel. +52 442 2119900 ext. 1527, cgarcia@qro.cinvestav.mx

**Synthesis and characterization of  $\text{Pr}_{0.9}\text{Sr}_{0.1}\text{Ni}_{0.6}\text{Fe}_{0.4}\text{O}_3$  perovskite as cathode material for intermediate temperature solid oxide fuel cell**

**I.B. Dzul-Bautista<sup>a,\*</sup>; N. Hernández<sup>a</sup>; R. Cienfuegos-Pelaes<sup>a</sup>; I. Ruiz de Larramendi<sup>b</sup>**

<sup>a</sup>Centro de Innovación, Investigación y Desarrollo en Ingeniería y Tecnología, Facultad de Ingeniería Mecánica y Eléctrica, Universidad Autónoma de Nuevo León, Km. 10 Autopista al Aeropuerto Internacional de Monterrey, PIIT Monterrey, C.P. 66629, Apodaca, Nuevo León.

<sup>b</sup> Universidad del País Vasco (UPV/EHU), Barrio Sarriena, s/n 48940 Leioa, Vizcaya, España

**ABSTRACT**

$\text{Pr}_{0.9}\text{Sr}_{0.1}\text{Ni}_{0.6}\text{Fe}_{0.4}\text{O}_3$  (PSNF) material with perovskite structure was prepared by citrate–nitrate sol-gel route. DSC/TG showed a major exothermic event approximately 400 °C attributed to removal of organic material and semicrystallization, the material was calcined at 850 °C since the thermogram did not show change in mass or any thermal event is observed over this temperature. X-ray diffraction data was used to determine orthorhombic symmetry with space group  $Pbnm$  and cell parameters by FullProf software analysis; additionally crystal size was calculated by Scherrer equation resulting 24 nm. Electrical conductivity and electrochemical measurement were performed. PSNF material fulfilled the requirements of electrical conductivity ( $129 \text{ Scm}^{-1}$  at 850 °C). The Area Specific Resistance (ASR) of PSNF cathode measured on a  $\text{Sm}_{0.2}\text{Ce}_{0.8}\text{O}_{1.9}$  (SDC) electrolyte reached a relatively low value of  $0.13 \text{ } \Omega/\text{cm}^2$  at 850 °C. PSNF and SDC presented similar thermal expansion coefficient (TEC) measured. PSNF is a promising candidate for use as cathodic material in solid oxide fuel cell.

**Keywords:** Perovskite, Cathode, Solid oxide fuel cell

\* Corresponding author:

Isabel Berenice Dzul Bautista, +52 8180781150, isab\_2@hotmail.com

**Effect of porosity on IEC and water distribution for sulfonated  
poly(styrene-co-acrylic acid) PEM copolymer**

**L. Melo<sup>a</sup>; R. Benavides<sup>a</sup>; G. Martínez<sup>a</sup>; D. Morales<sup>a</sup>; M.M.S. Paula<sup>b</sup>; L. Da Silva<sup>b</sup>**

<sup>a</sup>Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna H. 140, Saltillo, Coahuila, México.

<sup>b</sup>Universidade do Extremo Sul Catarinense (UNESC), Av. Universitária, 1105 - Cx.P. 3167, Criciúma, SC. Brazil, 88.806-000

**ABSTRACT**

Polystyrene-acrylic acid copolymers were synthesized by radical solution copolymerization reactions involving two different crosslinking agents (divinyl benzene-DVB or trimethylol propane trimethacrylate-TMPTMA) and further sulfonated with sulfuric acid catalyzed with silver sulfate. Casting procedures to obtain membranes consisted in dissolving copolymers in THF and the mixture THF/DMSO (DMSO at two levels: 55 and 110 %mol) followed by slow evaporation. Copolymers are miscible in the solvents mixture despite are immiscible in neat DMSO. Characterization of membranes was carried out by ion exchange capacity (IEC) measured by titration, water uptake (WU) measured gravimetrically, gas chromatography with mass detector (GC-MS) for measuring residual DMSO and scanning electron microscopy (SEM) to observe membrane structure. SEM images show considerably higher amount of pores for the THF/DMSO casted membranes, comparing with the ones obtained from neat THF. High amount of DMSO in the solvent mixture enhance IEC values (from 0.14 to 0.55 meq/g for DVB copolymer and from 0.08 to 0.9 meq/g for TMPTMA copolymer) as well as WU (from 15 to 105 % and from 14 to 139 % respectively) with no residual DMSO as measured by GC-MS. These important differences do not correlate with a relatively small difference in dimensional changes after membrane hydration (from 2.5 to 8 %). The pore formation is a consequence of differences in molecular weights between THF and DMSO (72 and 78 g/mol respectively) but most important to evaporation temperature differences (66 and 189 °C respectively). The general effect of using a solvent mixture for the casting procedure is the promotion of differences in the microscopic hydrophilic/hydrophobic domains into the molecular structure of the polyelectrolyte. Once the THF evaporates, DMSO itself has no salvation possibilities and remains longer into the copolymer matrix as bubbles, leaving pores after its final extraction. IEC and WU values increase due to the higher possibilities for water to remain into de membranes after hydration, since pores allow more water inside with lower dimensional changes. The latter in turn will allow protons to exchange easily, enhancing IEC value.

**Keywords:** Porosity, IEC, Water uptake

\* Corresponding author:

Roberto Benavides, +52(844)438 9830 xt. 1322, fax: +52(844)438 9839, roberto.benavides@ciqa.edu.mx

**Polystyrene-co-acrylic acid proton exchange membranes:  
morphology and mechanical properties**

**L. Melo<sup>a</sup>; R. Benavides<sup>a</sup>; G. Martínez<sup>a</sup>; M.L. López<sup>a</sup>; MMS Paula<sup>b</sup>; L. Da Silva<sup>b</sup>**

<sup>a</sup>Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna H. 140, Saltillo, Coahuila, México.

<sup>b</sup>Universidade do Extremo Sul Catarinense (UNESC), Av. Universitária, 1105 - Cx.P. 3167, Criciúma, SC. Brazil, 88.806-000

**ABSTRACT**

Two random copolymers of poly(styrene-co-acrylic acid) (PS-AA) were synthesized in solution (diethylbenzene) by radical polymerization and partially crosslinked by adding, either the trifunctional monomer trimethylol propane trimethacrylate (TMPTMA) or the difunctional monomer divinylbenzene (DVB) to improve mechanical resistance. Crosslinked copolymers were also dissolved in dichloromethane and sulfonated with theoretical molar quantities of sulfuric acid ( $\text{H}_2\text{SO}_4 = 170\%$ ) and two different amounts of silver sulfate ( $\text{Ag}_2\text{SO}_4 = 0.11$  or  $0.055\%$ ) as a sulfonation reaction catalyst. Materials (neat and sulfonated) were dissolved in three different solvent compositions: copolymer+THF, copolymer+THF+55%DMSO and copolymer+THF+110%DMSO and then membranes prepared by casting from them. Membranes were fully activated by immersing them in  $\text{HNO}_3$ , followed by  $\text{H}_2\text{O}_2$  and finally in  $\text{H}_2\text{SO}_4$ . Thermomechanical Analysis (TMA), Ionic Exchange Capacity (IEC), Water Uptake (WU) and Scanning Electron Microscopy (SEM) were used to evaluate membranes. Addition of DMSO to THF as a mixture of solvents during casting procedure for the same sulphonated copolymer has an important increment on IEC and WU results. However, mechanical resistance measured by flexure modulus (ASTM D790) in a TMA is considerably reduced. SEM images show almost no pores in the membranes casted from THF alone, while increasing the amount of DMSO mixed with THF for casting, an increment in porosity is clearly seen. 55% DMSO materials have an important amount of pores, but for the 110% DMSO membranes, SEM images show them side-by-side. Such phenomenon is responsible for the lowest mechanical property (brittleness), as seen by TMA results for the same membranes. In general, the mixture of solvents THF+DMSO enhance water uptake and ionic properties but reduce mechanical resistance of PS-AA copolymers.

**Keywords:** Copolymers, Casting, Flexure modulus, Porosity

\* Corresponding author:

Roberto Benavides, +52(844)438 9830 xt. 1322, fax: +52(844)438 9839

Roberto.benavides@ciqa.edu.mx





**Statistical analysis of the microstructure of a proton exchange membrane  
fuel catalyst layer**

**J. Ramírez<sup>a</sup>; R. Barbosa<sup>b,\*</sup>; E. Escobedo<sup>a</sup>; D. Pacheco<sup>a</sup>; B. Escobar<sup>a</sup>**

<sup>a</sup>Unidad de Energía Renovable, Centro de Investigación Científica de Yucatán, C 43 No 130, Chuburná de Hidalgo, Mérida, Yucatán, México, 97200.

<sup>b</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Quintana Roo, México, 77019.

**ABSTRACT**

The deposition technique and the composition and structure of the elements that make up the catalyst layer (CL) of a proton exchange membrane fuel cell (PEMFC), affect the final CL structure. This in turn, changes the overall response of the PEMFC. The CL is defined as a random heterogeneous material composed of different phases: the catalyst is typically platinum (Pt), the supporting material most commonly used is carbon (C), the ionomer is a polymer named nafion®. Furthermore, the CL needs to be porous to allow the access of reactant gases and to enable an effective water balance. Locating a complete description of the microstructure of a real electrode is not an easy job. The main reasons are that the CL shows non-uniform microstructures at different scales. By techniques of stochastic reconstruction, finite volume method and scanning electron microscopy (SEM) we can quantify the microstructural changes. The principal objective of this work is the study of the CL microstructure to identify and quantify changes at different scales. By SEM, image processing and statistical characterization techniques, we find two representative scales and their correlation functions. Therefore, two different manufacturing techniques were carried out with electro-spray deposition technique: 1) catalyst deposited on the membrane and; 2) catalyst deposited on the gas diffusion layer (GDL). Finally, by applying the continuity equation in a medium discretized by finite control volumes, the conduction efficiency was determined [R. Barbosa, et. al., J. Power Sources 2011; 196: 1248–1257].

**Keywords:** Correlation functions, Heterogeneous media, Electro-spray, Catalyst layer

\* Corresponding author:

R. Barbosa, tel. +52 (983) 8350300 - Ext: 244, fax. +52 (983) 8329656, romelix1@gmail.com

**Comparative study of different carbon supported  $\text{Fe}_2\text{O}_3/\text{Pt}$  catalysts  
for oxygen reduction reaction**

**M.M.Tellez-Cruz<sup>a</sup>; M.A. Padilla-Islas<sup>a</sup>; O. Solorza-Feria<sup>a\*</sup>**

<sup>a</sup>Departamento de Química, Centro de Investigación y Estudios Avanzados del IPN Av. IPN 2508, Col. San Pedro Zacatenco, A. Postal 14-740, 07360 México D.F., México. <sup>\*</sup>Tel: 011 +52 +55 5747-3715 ; e-mail: osolorza@cinvestav.mx

**ABSTRACT**

The prohibitive cost of platinum for catalyzing the cathodic oxygen reduction reaction (ORR) has hampered the widespread use of polymer electrolyte fuel cells. To reduce the amount of the Pt used in fuel cells, one approach is to introduce an additional metal to form Pt based alloy as a substitute for pure Pt. Another of the challenges that a catalyst is facing is, the right dispersion of this in the porous matrix that supports it, commonly carbon. To achieve this goal carbon functionalization procedures must be performed to be a guide for growth catalyst, improving the dispersion, allow use a smaller amount of catalyst to achieve higher electrochemically active area.

We report here effects of two kinds of functionalized carbon supports (carbon vulcan and carbon black pearl) in the activity of  $\text{Fe}_2\text{O}_3/\text{Pt}$  catalyst for oxygen reduction reaction (ORR) in acid media. The core was synthesized by chemical reduction with  $\text{NaBH}_4$  of the precursor salt, while the shell was deposited by galvanic displacement in the surface atoms of  $\text{Fe}_2\text{O}_3$  in the particles. The material was characterized by XRD, TEM and EDAX. The electrochemical performance of  $\text{Fe}_2\text{O}_3/\text{Pt}/\text{C}$  is evaluated by cyclic voltammetry, CO stripping and RDE.

Consequently, the results indicate that the  $\text{Fe}_2\text{O}_3/\text{Pt}/\text{C}$  catalyst could be used as a more economically viable alternative for the ORR of PEMFCs.

**Keywords:**  $\text{Fe}_2\text{O}_3/\text{Pt}/\text{C}$  catalyst, Oxygen reduction reaction, Core-shell

\* Corresponding author:

O. Solorza-Feria, tel. +52 55 57473800, osolorza@cinvestav.mx

**New advanced 2D NiAu@Pt nanolayers with high electrocatalytic activity  
for the oxygen reduction reaction**

**F. Godínez-Salomón<sup>a,b</sup>; D. Bahena<sup>a</sup>, R. McFeron<sup>b</sup>, O. Solorza-Feria<sup>a</sup>; C. P. Rhodes<sup>\*b</sup>**

<sup>a</sup>Centro de Investigación y estudios Avanzados del IPN, Depto. Química, Av. IPN 2508. A. P. 14-740, CP. 07360, México-D.F. México.

<sup>b</sup>Department of Chemistry and Biochemistry, Texas State University, 601 University Dr. San Marcos Tx 78666.

**ABSTRACT**

Recently two-dimensional (2D) materials with nanosheet-like structures have gained world-wide attention for use in many different technological applications as sensors, catalysts, energy conversion and storage. Due to quantum confinement, surface controlled structures, and the ability to tune the structure and number of atomic layers of 2D materials, it is possible to achieve unprecedented properties not seen in their bulk counterparts. In this context, many efforts have been devoted to the development of new synthetic routes that control the atomic structure, electronic structure, surface energy and electrical, optical, magnetic and electrocatalytic properties of 2D materials. Since the discovery of graphene by Novoselov et al. in 2004, significant efforts have been aimed at the study of 2D transition metal oxides and dichalcogenides in addition to graphene. In contrast, very few reports that utilize metallic 2D structures have been reported, particularly for hydrogen fuel cell applications. The use of 2D materials, may provide highly reactive edge and surface states that provide improved electrocatalytic activity, particularly for the sluggish oxygen reduction reaction (ORR). Previous studies carried out in our group, have demonstrated the potential of Ni@Pt core-shell nanoparticles to provide improved ORR catalysts for fuel cells, however further improvements in the stability of the materials are still needed. Two-dimensional NiAu@Pt alloy were synthesized and characterized to provide ORR electrocatalysts with improved durability, cost and performance.

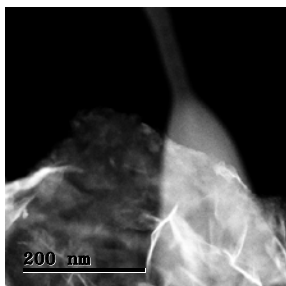


Fig. 1. Scanning transmission electron microscopy images of ultrathin NiAu nanosheet used as core.

**Keywords:** Two dimensional nanosheets, Core-shell, Oxygen reduction reaction, Fuel cell, Advanced materials

\* Christopher P. Rhodes; cprhodes@txstate.edu, (1-512) 245 6721.

**Development of an electrolysis stack type solid polymer electrolyte**

**E. Sosa-Caamal<sup>a</sup>; R. Barbosa<sup>b</sup>; B. Escobar<sup>c</sup>; G. Rodriguez- May<sup>a</sup>; Ysmael Verde<sup>d</sup>;  
J. C. Cruz\***

<sup>a</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 77013, México

<sup>b</sup>Universidad de Quintana Roo, Boulevard Bahía, s/n, Chetumal, Quintana Roo 77019, México

<sup>c</sup>Cento de Investigación Cietífica de Yucatán, A.C., Calle 43 No. 130 Colonia Chuburná de Hidalgo, Mérida, Yucatán 97200, México

<sup>d</sup>Instituto Tecnológico de Cancún, Av. Kabah km 3, Cancún, Quintana Roo 77500, México

**ABSTRACT**

A new generation of highly efficient and non-polluting energy conversion and storage systems was vital to meeting the challenges of global warming and the finite reality of fossil fuels. One of these is the hydrogen , however , this is not free as such in nature. Because of this there are different ways to get this fuel mediante electrochemical processes. One such process is carried out in an electrolyser. Aelectrolizer is an electrode system for separation the hydrogen and oxygen molecules applying a potential difference for optencion hydrogen and oxygen with purity of about 99% . In this work, it was made design and characterization of an electroyzer stack for 4 cell with polimeric membranes PEM at room temperature. A stack was building of circular pattern with acrylic material in order to observe the phenomena occurring in the system. The material was used, IrO<sub>2</sub> catalys anode and at the cathode Pt/C were deposited on a membrane of Nafion 115. The materials were deposited by hot spray technique, the IrO<sub>2</sub> catalys loading of ~1 mg cm<sup>-2</sup> and 0.5 mg cm<sup>-2</sup> of Pt/C (30% wt, Pt) as hydrogen electrode. The stack was tested 1.6 V to 2 V per cell. The electrical resistance of the electrolyte were evaluated by electrochemical impedance spectroscopy of each cell. A stack of electrolyzers for science in schools and higher secondary education was obtained.

**Keywords:** Electrolyzer, IrO<sub>2</sub>, Stack

\* Corresponding author: Dr Julio Cesar Cruz Argüello, 9831043002,México, jcruz@itchetumal.edu.mx

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Development of polymer solid electrolyte type fuel cell stack of H<sub>2</sub>/O<sub>2</sub>**

**E.F. Barbosa-Mex<sup>a</sup>; R. Barbosa<sup>b</sup>; B. Escobar<sup>c</sup>; G. Rodriguez-May<sup>a</sup>; Ysmael Verde<sup>d</sup>;  
J.C. Cruz<sup>a\*</sup>**

<sup>1</sup>Universidad de Quintana Roo, Boulevard Baha s/n, Chetumal, Quintana Roo 77019, México

<sup>2</sup>Centro de Investigación Científica de Yucatán, A.C., Calle 43 No. 130 Colonia Chuburná de Hidalgo, Merida, Yucatan 97200, Mexico

<sup>3</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 77013, Mexico

<sup>4</sup>Instituto Tecnológico de Cancun, Av. Kabah km 3, Cancun, Quintana Roo 77500, México

<sup>5</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 77013, Mexico

**ABSTRACT**

A single fuel cell voltage is quite small, about 0.7 Vcd, a useful power. This means that in order to produce one useful voltage greater, many fuel cells must be connected in series. Such grouping of fuel cell is known as stack. The most obvious way the edge of the cathode of the next cell, along the entire line. In this work, the stack of four fuel cells of the H<sub>2</sub>/O<sub>2</sub> polymer solid electrolyte type fuel cell, was developed for obtaining educational kits with nanomaterials dimensions of 25 cm<sup>2</sup> geometric area. At the anode and cathode Electrocatalyst used Pt/C (30%wt), catalyst loading 0.5 mg cm<sup>-2</sup>. Therefore the deposits were made with materials through the hot spray system temperatura environment. The development of liquid and gas fuel cells to increase effectiveness and efficiency that currently have alkaline batteries for use in portable and digital systems. The design construction and evaluation of fuel cell hydrogen and oxygen through the electrooxidación of the same stimulated a transportable means of energy of high density to low surface area. As the common means of electrooxidación of gases lead an energy density higher than common batteries. The application of new technologies through the use of nanomaterials in the energy industry will be a relevant point in the near future. A stack of fuel cell for science in schools and higher secondary education was obtained.

**Keywords:** Fuel cell, Stack, Membrane

\* Corresponding author: Dr. Julio César Cruz Argüello 9831043002, México, jcruez@itchetumal.edu.com



**Thermo mechanical system for manufacturing fuel cell electrodes**

**L.A. Soto-Ramirez<sup>a</sup>; J.C. Cruz<sup>a</sup>; B. Escobar<sup>b</sup>; R. Barbosa<sup>c\*</sup>**

<sup>a</sup>Instituto tecnológico de Chetumal, AV.Insurgentes s/n, Chetumal, Quintana Roo 77013, México

<sup>b</sup>Centro de Investigación científica de Yucatán, A.C., Calle 43 No. 130 Colonia Chuburná de Hidalgo, Mérida, Yucatán 97200, México.

<sup>c</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Quintana Roo, 77019, México.

**ABSTRACT**

The thermo mechanical system is a recognized method to expedite or improvement in manufacturing micro fuel cell electrodes because it facilitates the assembly process without having lost in the materials of electrodes and having micro fuel cells with maximum efficiency. The thermo mechanical system consists of a hydraulic press (test press multi 25-i), which is adapted a temperature control system, the temperature is applied through four steel plates, these are assembled in the base of the press forming a type in capped, to avoid heat loss during treatment, within it will be the micro electrode fuel cell, these steel plates each has on mounted a resistance heat which are controlled by the control system temperature, temperature control has a range of 0° C to 130° C that when a voltage is applied to the heat generating thermistors are in turn through the heat transmitting plate electrode fuel cell micro, at the same instantly applies a pressure to the press that has a range of 1-25 kg / cm<sup>2</sup>, the pressure varies during a time of 5 minutes, which is the estimated time for the entire assembly, since it is the time where the pores and solvent removal in already completely eliminated, and the fuel cell have an electrode with an efficiency of 100% and the fuel cell will not inefficiency losses in the electrode. In this project the assembled micro fuel electrode in the same press in order to avoid mismatches in the materials of the micro electrode is proposed.

**Keywords:** Thermo mechanical, Assembly process, Control system

\* Corresponding author:

Dr. Gliserio Romeli Barbosa Pool, +983 156 6032, romelix1@gmail.com

**Development of micro electrodes by alternative system**

**F.Torres-Torres<sup>a</sup>; J. C. Cruz<sup>a</sup>; B.Escobar<sup>b</sup>; R.Barbosa<sup>c\*</sup>**

<sup>a</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 77013, México

<sup>b</sup>Centro de Investigación Científica de Yucatán, A.C., Calle 43 No.130 Colonia Chuburná de Hidalgo, Mérida, Yucatán 97200, México

<sup>c</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Quintana Roo 77019, México

**ABSTRACT**

A micro electrode fuel cell is a system capable of being inserted into a cell. The micro electrodes have many potential uses and applications. Currently it is looking to be even smaller for transport and to increase the efficiency of the discharging process. In this paper it is proposed that the micro electrode fuel cell be developed as an alternative system with a proposed construction that will have as main objective facilitating or improving the assembly process, as this part of the process is where most problems and human errors . Unlike this method, the assembly of the micro electrode won't have this type of problem as it doesn't have to move from one place to another because this method does all the assembly at the same time and not in stages. In the heat treatment process of the fuel cell, it looks to diminish the time possible for delivering equal or better results with material uniformity to treat the fuel cells: such as to deposit the materials in the micro cracks and pores. This is why we apply a temperature to completely dissolve the material and to remove microelectrode micro cracks that would prevent contact between the electrodes when activating the membrane. Similarly, the micro fuel cell electrode can be designed from construction material use and deliver cargo on the power system where it is installed. Furthermore, the micro electrode look as compact as possible and efficient discharge time.

\* Corresponding author:

Dr Gliserio Romeli Barbosa Pool , 983 156 6032  
romelix@gmail.com



**An optimization study of the electrophoretic deposition parameters to prepare PEMFC electrodes using non-asymmetric AC electric field**

**W.J. Pech-Rodríguez<sup>a</sup>; D. González-Quijano<sup>a</sup>; G. Vargaz-Gutierrez<sup>a,b</sup>;**  
**J.I. Escalante-García<sup>a,b</sup>; F.J. Rodríguez-Varela<sup>b,c,\*</sup>**

<sup>a</sup>Ingeniería Metalúrgica e Ingeniería Cerámica

<sup>b</sup>Sustentabilidad de los Recursos Naturales y Energía

<sup>c</sup>Programa de Nanociencias y Nanotecnología

Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe, Ramos Arizpe, Coahuila, C.P. 25900, México

**ABSTRACT**

PEM Fuel Cell electrodes were fabricated by electrophoretic deposition (EPD) under Non-Asymmetric AC electric field, by deposition of a catalytic layer of home-synthesized Pt/C nanoparticles on commercial carbon cloth as support. The experiments were carried out based on a L9 orthogonal Taguchi experimental design array with four factor control at 3 levels. The effect of various parameters such as applied voltage, deposition time, asymmetric factor and Nafion content has been studied. The obtained layers were characterized by Scanning Electron Microscopy to investigate the dispersion of the catalyst. The results indicated that EPD is an effective method to fabricate PEM fuel cell electrodes with thin and homogeneous catalytic layer. Electrochemical studies of the EOR in acid media demonstrated a high electrocatalytic activity for the EOR of the electrodes fabricated using the EPD technique.

**Keywords:** Electrophoretic deposition, Fuel cell electrodes, Ethanol oxidation reaction, Parameters optimization

\* Corresponding author:

F.J. Rodríguez-Varela, Phone number: +52(844)438-9600 Ext. 8526, E-mail: javier.varela@cinvestav.edu.mx

**Specific and mass activities of Ni-Pd nanoparticles for the oxygen reduction reaction in acid medium**

**C.V. Tinoco-Muñoz<sup>a,\*</sup>; J.L. Reyes-Rodríguez<sup>b</sup>; D. Uribe-Bahena<sup>c</sup>;  
J.G. Cabañas-Moreno<sup>a</sup>; O. Solorza-Feria<sup>b</sup>**

<sup>a</sup> Programa Nanociencias y Nanotecnología, Centro de Investigación y Estudios Avanzados, CINVESTAV-IPN.

<sup>b</sup> Departamento Química, CINVESTAV-IPN.

<sup>c</sup> L.A.N.E.-CINVESTAV-IPN. Av. IPN 2508, Col. Zacatenco, 07360, México D.F., México.

**ABSTRACT**

The goal of the present study was to develop an active nanocatalyst as well as exploring the benefits to produce an alloy free of platinum for the oxygen reduction reaction. The Ni-Pd catalyst was synthesized by using a methodology previously developed in our group of research, which consisted of two consecutive steps: the reduction of the Ni(Acac)<sub>2</sub> precursor to metallic Ni with sodium borohydride (NaBH<sub>4</sub>), followed by the formation of the alloy by the galvanic displacement of Ni surface atoms by Pd atoms using ethylene glycol as the dispersion medium. Powder of the synthesized nanocatalyst was dispersed in 20 wt.% Carbon Vulcan XC-72R previously functionalized with ethanolamine. The electrochemical study was performed in a typical three electrodes electrochemical cell in 0.1 M HClO<sub>4</sub> electrolyte. The physical characterization was performed by X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM). Electrochemical results show that Ni-Pd electrocatalyst has an electrochemical active surface area, (ECSA) of about 70 m<sup>2</sup>/g. Results of the ORR conducted to specific activity (SA = 0.106 mA/cm<sup>2</sup><sub>cat</sub>) and mass activity (MA = 0.320 A/mg<sub>cat</sub>), both evaluated at 0.9 V vs. NHE. These preliminary results are low compared to commercially available Pt catalyst (Pt-E TEK; ESCA = 77.11 m<sup>2</sup>/g, SA = 0.21 mA/cm<sup>2</sup> and MA = 0.180 A/mg<sub>cat</sub> @ 0.9 V vs. NHE). However, probably the catalytic activity could be improved by incorporation of a reduced Pt content in the Ni-Pd catalyst.

**Keywords:** Oxygen reduction reaction, Catalyst Ni-Pd, Alloy nanoparticles

\* Corresponding author:

C. V. Tinoco-Muñoz, (55) 57473800 Ext. 4473, ctinoco@cinvestav.mx; clautm3@gmail.com

**CoTiO<sub>3</sub> deposited by laser ablation on a commercial alkaline membrane:  
electrochemical performance for the ORR reaction in alkaline media**

**R. Basurto Sánchez<sup>a</sup>; T. Romero Castañón<sup>b</sup>; L. Escobar Alarcon<sup>c</sup>;  
M. A. García Contreras<sup>a</sup>; J. Bonifacio Martínez<sup>a</sup>; E. Ordoñez-Regil;  
S. M. Fernández Valverde\***

<sup>a</sup>Depto. de Química, Instituto Nacional de Investigaciones Nucleares, A.P. 18-1027, Mexico D.F. C.P.11801, Mexico. Tel. 5553297200 ext 12277 <sup>b</sup>Gerencia de Energías No Convencionales, Instituto de Investigaciones Eléctricas (IIE), Av. Reforma 113, Col. Palmira 62490, Cuernavaca, Mor., México

**ABSTRACT**

Oxygen electrochemistry is at the basis of renewable energy technologies. Yet, one of the major challenges is the search of stable and high efficiency membranes-electrocatalyst for alkaline fuel cells. The objective of this work was to test the pulsed laser deposition (PLD) technique to prepare an assembly membrane-electrode with a commercial zirconium membrane and CoTiO<sub>3</sub> electrocatalyst obtained by Mechanical Alloying and tested for the Oxygen Reduction Reaction (ORR) in alkaline media. CoTiO<sub>3</sub> was synthesized by MA technique mixing Co<sub>3</sub>O<sub>4</sub> and commercial titanium oxide. The physical and chemical characterization was done by: XRD in a Siemens D5000, SEM and EDX in a JEOL-JSM-5900 LB with an EDAX microprobe. Binding energies were determined in a Thermo Scientific K-Alpha XPS, BET analysis and pore diameter was obtained in a Bel Sorp max Bel Japan Inc. The ORR was performed in 0.5 M KOH solution, in a conventional three electrode cell, the reported current densities are referred to the geometric surface area of working electrodes. The specific area was  $2.81 \times 10^{-2} \text{ m}^2 \text{ g}^{-1}$  and the total pore volume was  $8.13 \times 10^{-4}$ , the current density was  $6.5 \text{ mA cm}^{-2}$  at 0.8 mV and 1600 rpm. This value was constant for different experiments therefore CoTiO<sub>3</sub> is stable for the ORR. The Kinetic parameters obtained were:  $I_0$   $5.96 \times 10^{-4} \text{ mA cm}^{-2}$ ,  $\alpha$  0.25 and  $b$   $159 \text{ mV dec}^{-1}$ . Ti(III), Ti(IV), Co(III) and Co(II) were determined by XPS, the XRD pattern corresponded to CoTiO<sub>3</sub> structure. This material was deposited on the zirconium membrane by PLD, CoTiO<sub>3</sub>-zirconium membrane assembly was tested in the same experimental conditions described before for the ORR and stability. In conclusion it was confirmed that: the assembly has good performance for the ORR in alkaline media. The characterization in a single fuel cell is the next research.

**Keywords:** ORR in alkaline media, Alkaline membranes, CoTiO<sub>3</sub>, Laser deposition

\*Sulma M. Fernández-Valverde, +52 01 55 53 29 72 00 ext. 12277: [sulma.fernandez@inin.gob.mx](mailto:sulma.fernandez@inin.gob.mx)

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Electrocatalytic Oxygen Reduction Reaction (ORR) on nanostructured  
Pt-NiTiO<sub>3</sub>/C catalyst in alkaline media**

**A. Hernández-Ramírez<sup>a</sup>; M. E. Sánchez-Castro<sup>a,b</sup>; Kalasapurayil Kunhiraman Aruna<sup>c</sup>;  
Palanisamy Karthikeyan Manoharan<sup>c</sup>; F. J. Rodríguez-Varela<sup>a,b,\*</sup>**

<sup>a</sup>Programa de Nanociencias y Nanotecnología, Cinvestav Unidad Saltillo, Av. Industrial Metalúrgica No. 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coah., México, 25900.

<sup>b</sup>Grupo de Sustentabilidad de los Recursos Naturales, Cinvestav Unidad Saltillo, Av. Industrial Metalúrgica No. 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coah., México, 25900.

<sup>c</sup>Electrochemical Energy Materials Laboratories, Nanotech Research Facility, PSG Institute of Advanced Studies, Coimbatore, India 641 004

**ABSTRACT**

The catalytic activity for the ORR on carbon supported Pt-NiTiO<sub>3</sub> catalyst was evaluated in 0.5 M KOH electrolyte. NiTiO<sub>3</sub> nanoparticles were synthesized via a wet-chemical method. Then, 20% Pt-NiTiO<sub>3</sub> catalysts (Pt:NiTiO<sub>3</sub> ratio of 1:1, 2:1 and 3:1 at.%) were obtained by the microwave assisted polyol method. TEM analysis showed homogeneously dispersed nanoparticles on the carbon support with a narrow particle size distribution of around 2-3 nm. The titanate-containing catalysts showed a high catalytic activity for the ORR. Moreover, these cathodes showed enhanced tolerance to methanol and ethanol, compared to Pt/C.

**Keywords:** Pt-NiTiO<sub>3</sub>/C catalyst, Oxygen reduction reaction, Alkaline media, Tolerance to organic molecules

\* Corresponding author:

F.J. Rodríguez-Varela, Phone number: +52(844)438-9600 Ext. 8526, E-mail: javier.varela@cinvestav.edu.mx



**Evaluation of the Bismuth content effect on cathodic catalysts for PEM fuel cells**

**O. X. Guerrero-Gutiérrez<sup>a</sup>; F. A. Bugueño-Bucio<sup>b</sup>; O. Solorza-Feria<sup>a,\*</sup>**

<sup>a</sup>Departamento de Química. Centro de Investigación y de Estudios avanzados, CINVESTAV-IPN. Av. IPN 2508, Zacatenco. México D.F.

<sup>b</sup>Facultad de Química. Universidad Nacional Autónoma de México. UNAM.

**ABSTRACT**

Fuel Cells are one of the most promising alternatives for producing clean energy. However, there are commercial bottlenecks for expanding Proton Exchange Membrane Fuel Cells (PEMFC) use and application. One of them is the high cost and unstability of the catalysts. Pt is among the best catalyst for fuel cells. Preparing materials with less Pt content, to decrease catalyst costs, has shown to increase the electrocatalytic activity in some cases. This work focuses on evaluating the effect of Bi content on Pt and Pd catalysts. Since Mexico is one of the largest Bi producers, it is an objective to add value to this metallic national product. In this work, Bi has been incorporated to the fuel cell's Pt and Pd cathodic catalyst, which are known to have good activity towards the Oxygen Reduction Reaction (ORR). Carbon supported BiPt nanoparticles were prepared by different synthetic methods to evaluate their specific and mass ORR activities. Catalytic activities were measured via a thin film on a rotating disk electrode, getting the kinetic current generated at 0.9V and normalizing it with the electrochemical surface area (ECSA) and the mass of the catalyst deposited on the electrode. ECSA was measured by adsorbing a CO monolayer on the catalyst and measuring the charge generated from its oxidation. Cyclic voltammograms of Bi@Pt results show a non-Pt-like behaviour, low ECSA ( $<1 \text{ m}^2/\text{g}_{\text{Pt}}$ ) and a very poor ORR mass activity ( $<10 \text{ mA}/\text{mg}_{\text{Pt}}$ ) in acidic media when compared with commercially available Pt nanoparticles ( $65 \text{ m}^2/\text{g}_{\text{Pt}}$ ;  $100 \text{ mA}/\text{mg}_{\text{Pt}}$ ). Pd and Pt with Bi were prepared to evaluate the impact Bi has on the ORR activity. The  $\text{Pt}_{90}\text{Bi}_{10}$  catalyst shows a decrease in mass activity and ECSA ( $33 \text{ mA}/\text{mg}_{\text{Pd}}$  and  $13 \text{ m}^2/\text{g}_{\text{Pt}}$ ) but an increase in specific activity ( $264 \mu\text{A}/\text{cm}^2_{\text{Pd}}$ ) in respect to its Bi-free counterpart ( $50 \text{ mA}/\text{mg}_{\text{Pt}}$ ,  $45 \mu\text{A}/\text{mg}_{\text{Pt}}$  and  $112 \text{ m}^2/\text{g}_{\text{Pt}}$ ). The  $\text{Pd}_{90}\text{Bi}_{10}$  catalyst shows an increase in its activities ( $26 \text{ mA}/\text{mg}_{\text{Pd}}$  and  $160 \mu\text{A}/\text{mg}_{\text{Pd}}$ ) and a decrease in ECSA ( $16 \text{ m}^2/\text{g}_{\text{Pd}}$ ) with respect to its Bi-free counterpart ( $6 \text{ mA}/\text{mg}_{\text{Pd}}$ ,  $13 \mu\text{A}/\text{mg}_{\text{Pd}}$  and  $50 \text{ m}^2/\text{g}_{\text{Pd}}$ ).

**Keywords:** Nanomaterials, PEMFC, Fuel cell, ORR

\* Corresponding author:

Oscar Xavier Guerrero Gutiérrez, 57473800, ext. 4473, xguerrero@cinvestav.mx

**Analysis of the oxygen reduction reaction in core-shell nanoparticles**

**S. Prasertthdam<sup>a</sup>; G. Ramos-Sanchez<sup>b</sup>; and P. B. Balbuena<sup>a,\*</sup>**

<sup>a</sup>Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, USA

<sup>b</sup>Universidad Autónoma Metropolitana-Iztapalapa, Departamento de Química, 55-534, C.P. 09340 México, D.F., México

**ABSTRACT**

The improvement of the catalytic efficiency for the oxygen reduction reaction (ORR) is one of the most important challenges in low-temperature fuel cell technology. Platinum is the most active element for the ORR but its high cost and scarcity hinder the commercial implementation of fuel cells in automobiles. Pt-based alloys are promising alternatives to substitute platinum while maintaining the efficiency and life-time of the pure catalyst. However, the presence of an acid medium and oxidation of the surface impacts the activity and durability of the alloy catalysts through changes in its local composition. Dealloying is the selective removal of elements from an alloy. According to recent experimental reports dealloying taking place during the synthesis of ORR catalysts may yield remarkable activity enhancement by creating characteristic porous or hollow structures. However, the dealloying process that occurs during the fuel cell operation is enhanced by the concomitant presence of oxygen that promotes metal dissolution causing the degradation of the catalyst. In this work we present a first-principles computational analysis oriented to investigate activity and stability properties of alloy nanocatalysts. Two types of core-shell systems: Pt/Re/Ni, and Pt/FeCFe/Ni are analyzed using density functional theory and ab initio molecular dynamics simulations. Our initial studies identified the Pt/Re/Ni core-shell system as being promising for an enhanced ORR activity. In addition, our earlier analysis identified the Pt/FeCFe/Ni core-shell as an outstanding ORR electrocatalytic material not only due to its superior activity but also improved stability against dissolution in acid medium. Here we demonstrate how such nanoparticle core-shell structures have indeed excellent potential to perform well as ORR catalysts. In addition, the role of the catalyst support: carbon vs. graphene oxide and N-substituted graphene oxide is also elucidated.

**Keywords:** Hydrogen fuel cells, Nanomaterials, Core-shell electrocatalysts, Catalyst-support interaction

\* Corresponding author:

Perla B. Balbuena, 1-979-845-3375 (phone) and 1-979-845-6446 (fax number), balbuena@tamu.edu



**Electrocatalytic properties of Ni, Co and Ni-Co nanoparticles for  
hydrogen evolution reaction in alkaline medium**

**S. Citalán-Cigarroa\*; O. Solorza-Feria**

<sup>a</sup>Depto. Química, Centro de Investigación y de Estudios Avanzados del IPN A. Postal 14-740, 07360 México D.F., México.

**ABSTRACT**

Hydrogen has been recognized as a potential energy vector for the energy future. The production of high purity hydrogen is required in the development of fuel cell technology resulting of great interest the research and development of new materials with non-precious metals. The aim of this communication is to present the synthesis and characterization of Ni, Co and NiCo nanocatalysts prepared by High Energy Mechanical Milling (HEMM). The catalytic activity and stability of the electrocatalysts were evaluated by cyclic voltammetry, CV and linear scan voltammetry, LV using rotating disc electrode RDE technique, in a KOH 1M solution. Catalytic results indicate that NiCo present the highest activity for the hydrogen evolution reaction (HER). Microstructural analyses and composition of the nanoparticles were evaluated by X-Ray diffraction and used for phases identification. Morphology and chemical composition were determined by SEM, TEM and EDS. The average particle size of the NiCo was about 60nm with agglomerated spherical and homogeneous form with chemical composition in agreement with estimated values for the HEMM preparation.

**Keywords:** Hydrogen evolution reaction, High Energy Mechanical Milling, Nanomaterials, Cobalt, Nickel

\* Corresponding author: Tel. : + 52 55 57473800 ext. 4473, E-mail Address: scitalan@cinvestav.mx



**Synthesis and characterization Pt/WO<sub>3</sub> supported on CNT for oxygen reduction reaction**

**E. Oseguera<sup>a,b</sup>; C. Cortés-Escobedo<sup>a</sup>; R. de G. González-Huerta<sup>b\*</sup>**

<sup>a</sup>Centro de Investigación e Innovación Tecnológica del Instituto Politécnico Nacional, Cda. Cecati s/n, Col. Sta. Catarina, CP 02250 Azcapotzalco, D.F., Mexico

<sup>b</sup>ESIQIE-Instituto Politécnico Nacional, Laboratorio de Electroquímica y Corrosión, UPALM, CP 07738 DF, Mexico

**ABSTRACT**

In the recent years, extensive research work is being carried out and reported on improving the performance of catalysts for both anode and cathode of polymer electrolyte membrane fuel cell (PEMFC). The electrochemical performance of CNT supported Pt-WO<sub>3</sub> electrocatalysts was investigated. WO<sub>3</sub> was typically deposited from tungstate, the deposition of which is induced by a pH change according to the reaction  $\text{WO}_4^{2-} + 2\text{H}^+ \rightarrow \text{WO}_3 \cdot \text{H}_2\text{O}$  by adding HCl. Platinum nanocatalysts on tungsten have been synthesized and characterized as catalysts for oxygen reduction reaction in 0.5 mol dm<sup>-3</sup> H<sub>2</sub>SO<sub>4</sub> solution, at 25 °C. Pt nanoparticle-tungsten trioxide/multi-walled carbon nanotube (Pt-WO<sub>3</sub>/MWCNT) materials were synthesized by polyol method. These composite materials were employed as cathode electrocatalysts for oxygen reduction reaction (ORR). The surface morphology of the carbon nanotubes and the prepared catalysts was examined by scanning electron microscopy (SEM). The SEM images revealed the preferential growth of aligned MWCNTs. The support surface of Pt-WO<sub>3</sub>/MWCNT catalysts was characterised using Raman spectra. Their electrocatalytic properties toward the ORR were investigated in acid media using the rotating disk electrode (RDE) technique. The ORR activity of Pt-WO<sub>3</sub>/MWCNT was compared with that of commercial Pt/C catalyst. Pt/WO<sub>3</sub>/CNT catalysts exhibited better catalytic activity, expressed in terms of kinetic current density at the constant, in comparison with Pt/C catalyst.

Authors thank CONACYT to the Programa de Redes Temáticas (RTH2) projects 252003 and 249795; and IPN SIP multidisciplinary project 1683.

**Keywords:** Multi-walled carbon nanotubes, Polyol method, PEM fuel cell

\* Corresponding author: [rosgonzalez\\_h@yahoo.com.mx](mailto:rosgonzalez_h@yahoo.com.mx)

ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPALM, CP 07738 DF, Mexico

## **Modeling and design**

**First-principles studies of graphene for its application in PEMFC: A review**

**I. Pala-Rosas<sup>a,\*</sup>; H. Cruz-Martínez<sup>b</sup>; F. Montejo-Alvaro<sup>b</sup>**

<sup>a</sup>Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional, Unidad Profesional Adolfo López Mateos, México D.F., C.P. 07738.

<sup>b</sup>Programa de Doctorado en Nanociencia y Nanotecnología, CINVESTAV, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. C. P. 07360.

**ABSTRACT**

As consequence of several situations caused by human activities such as global warming, rapid increase of energy demand in the world and depletion of fossil fuel reserves; the assurance of clean and efficient energy sources is one of the greatest challenges to be faced. Therefore, research of new environment-friendly energy sources and their practical applications has attracted increasing attention. Among the proposed clean energy sources, the proton exchange membrane fuel cell (PEMFC) is one of the most promising technologies for the low temperature regime required for many applications. However, its commercialization is severely hampered by the low kinetic of the oxygen reduction reaction (ORR) and the extremely high cost of platinum. Hence, the major challenge is to develop new Pt-based or Pt-free catalysts with high activity, durability and lower costs. In this review, it is discussed the progress on the application of graphene as support material or metal-free catalyst using first-principles methods. Investigations of defect-free or defective graphene as support material for Pt, Pt-based, Pd-based catalysts have been developed using density functional theory (DFT). The Pt and Pt-based nanoparticles present lower adsorption energies on pristine graphene than on vacancy graphene. The Pt<sub>27</sub> cluster supported on pristine graphene presents an adsorption energy about -0.75 eV, much lower than -5.34 eV reported for the Pt<sub>27</sub> cluster on monovacancy graphene. For application of graphene as Pt-free catalyst, several studies on pure and M-doped graphene (M=nitrogen, boron, sulfur and transition metals) have been developed for the ORR mechanism. The oxygen adsorption energy on C<sub>70</sub>H<sub>22</sub> graphene is approximately -4.011 eV, similar to that reported for Pt<sub>79</sub> nanoparticles. The results show that doped-graphene can be a great candidate for the ORR in fuel cells.

**Keywords:** Defective-graphene, Doped-graphene, Transition metals, ORR mechanism, DFT

\* Corresponding author: Israel Pala-Rosas, +52 (55) 53189081, C.P. 07360, ipalar@hotmail.com

**A First-Principles study of Co-Ni@Pt Core-Shell electrocatalysts for the oxygen reduction reaction**

**H. Cruz-Martínez<sup>a,\*</sup>; E. Flores-Rojas<sup>a</sup>; P. Calaminici<sup>b</sup>;**  
**O. Solorza-Feria<sup>b</sup>**

<sup>a</sup>Programa de Doctorado en Nanociencia y Nanotecnología, CINVESTAV, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. C. P. 07360.

<sup>b</sup>Departamento de Química, CINVESTAV, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. C.P. 07360.

**ABSTRACT**

Proton exchange membrane fuel cells (PEMFCs) have been considered as one of the most promising clean and efficient electrochemical energy source. Pt-based nanocatalysts exhibit the highest specific and mass electrocatalytic activities for hydrogen oxidation on the anode and oxygen reduction reaction (ORR) on the cathode of polymeric fuel cells. However, the sluggish kinetics of the ORR and the high cost of the platinum (Pt) restrict the performance and commercialization of the PEMFCs. Novel types of catalysts have been developed to improve the ORR performance, reactivity and durability, but these problems still require further investigations. In this submitted research, Co<sub>16</sub>-Ni<sub>16</sub>@Pt<sub>8</sub> Core-Shell catalysts for the ORR were studied theoretically. All calculations were performed using the density functional theory (DFT) implemented in the deMon2k program. To determine the lowest-energy structures and spin multiplicity of the Co<sub>16</sub>-Ni<sub>16</sub> core, several structures were extracted from Born-Oppenheimer Molecular Dynamics (BOMD) trajectories. Subsequently, Pt atoms were distributed uniformly as shell on Co<sub>16</sub>-Ni<sub>16</sub> core. On Co<sub>16</sub>-Ni<sub>16</sub> and Co<sub>16</sub>-Ni<sub>16</sub>@Pt<sub>8</sub> structures O and O<sub>2</sub> were adsorbed to determine the adsorption energies and active sites for the ORR. Results show that Co-Ni core is favored for alloy structures and the O and O<sub>2</sub> adsorption energies on the Co<sub>16</sub>-Ni<sub>16</sub>@Pt<sub>8</sub> alloy-core-shell structures are favored for the ORR in PEM fuel cells.

**Keywords:** Adsorption energy, Active sites, BOMD, ORR

\*Corresponding author:

Heriberto Cruz-Martínez, +52 (55) 5747 3800, ext. 4411, C.P. 07360. hcruz@cinvestav.mx

**Nb coating could enhance electrocatalytic performance and lifetime of Ni cathode in MCFC**

**A. Meléndez-Ceballos<sup>a,\*</sup>; S.M. Fernández-Valverde<sup>b</sup>; V. Albin<sup>a</sup>; A. Ringuedé<sup>a</sup>;  
M. Cassir<sup>a</sup>**

<sup>a</sup>Institut de Recherche de Chimie Paris, 11 rue Pierre et Marie Curie, F-75231 Paris Cedex 05, France.

<sup>b</sup>Depto. de Química, Instituto Nacional de Investigaciones Nucleares, A.P.18-1027, México D.F. C.P.11801, México

**ABSTRACT**

The Molten Carbonate Fuel Cell (MCFC) is a promising technology for high efficiency, sustainable electrical energy generation when powered by environmentally friendly fuels, such as biogas obtained from organic waste. One of the main problems concerning the MCFC is the cathode dissolution in the carbonate melt. The most common material used as cathode is nickel, which undergoes in situ oxidation and lithiation in the carbonate melt then nickel starts dissolving and after precipitates as metallic nickel onto the anode, causing a short-circuit between both electrodes through the electrolyte [1]. The current research proposes to solve the problem by the modification of the standard porous nickel cathode on which an ultra-thin layer of a metal oxide is deposited. For this, we used Atomic layer deposition (ALD) which is a chemical gas phase deposition technique developed in Finland in the 1970s by T. Suntola et al. [2]. In ALD, reactant gas pulses are separately introduced to reach the substrates to be coated. Growth is achieved through self-terminating surface reactions. Self-terminating means that only one monolayer of reactant gas species can be adsorbed to the surface during a pulse. With this technique reaching homogeneous, conformal and dense layers is possible. For this study Nb<sub>2</sub>O<sub>5</sub> was deposited onto nickel porous substrates and tested electrochemically in molten Li<sub>2</sub>CO<sub>3</sub>-K<sub>2</sub>CO<sub>3</sub> (62-38 mol %) eutectic at 650 °C during 230 h by means of chronopotentiometry and electrochemical impedance spectroscopy. After electrochemical characterization we could find a noticeable diminution in stabilization time towards oxygen reduction potential which clearly indicates the presence of some kind of catalytic process favoured by the presence of Nb on the cathode as reported before by Fang et al. [3]. Interestingly niobium oxides not only increase stack lifetime of Ni cathode but at the same time increasing the performance of the cathode in the MCFC.

**Keywords:** Molten Carbonate, Cathode Protection, Atomic Layer Deposition, Niobium Oxide

\* Corresponding author: Arturo Melendez Ceballos, +33 781 54 81 12, [arturo.melendez@chimie-paristech.fr](mailto:arturo.melendez@chimie-paristech.fr)

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**Design of a microfluidic system in a PEMFC cell**

**L. M. Ponce-Herrera<sup>a</sup>; G. Carbajal-De la Torre<sup>a\*</sup>; S.A. Gamboa-Sánchez<sup>b</sup>;  
K. Suarez-Alcantara<sup>c</sup>; M. Villagómez-Galindo<sup>a</sup>; M. A. Espinosa-Medina<sup>a</sup>**

<sup>a</sup>Universidad Michoacana de San Nicolás de Hidalgo, Edificio W, Ciudad Universitaria, Francisco J. Mújica S/N C.P. 58030, Morelia Michoacán, México, (443)3223500 ext. 3148, gctorre@umich.mx.

<sup>b</sup>Instituto de Energías Renovables, UNAM, Priv. Xochicalco S/N Temixco C.P. 62580, Morelos México.

<sup>c</sup>Instituto de Investigaciones en Materiales, UNAM, Ant. Carretera a Pátzcuaro 8701 C.P. 58341, Morelia Michoacán, México.

**ABSTRACT**

In this paper, it is presented the design and simulation of a prototype proton exchange fuel cell (PEMFC) micro scale with the ultimate goal of providing electricity in mobile applications which are almost indispensable in our daily use development. A numerical analysis was done by simulating computational fluid dynamics flow field using the COMSOL Multiphysics software, taking into consideration that our fluid flow with a physical model of creeping flow ( $Re < 400$ ), with which reached analysis to find the pressure distribution and flow rate within two proposals flow plate coil geometric arrangement, concluding that would be used for further study of the proposals, the cell that is located a discarded pressure drop due to the arrangement of the flow plate, thereby achieving optimal distribution of the reagents on the active surface of the fuel cell to the proposed scale.

Taking the final proposal plate electrochemical flow analysis was performed, making the assembly of the physical model using physical Secondary Current Distribution (SIEC) to assess the conservation of electric charge inside the cell and to evaluate conservation physical model species Reactive Flow in Porous Media (RFCs) for anode and cathode. To evaluate the electrical performance of the polarization curves given fuel cell were obtained, i.e. the graph cathode electric potential depending on the electric current density and the graph of the electrical power density based on the density electric current, with which the result and efficiency compared with the theoretical curve of a PEMFC cell polarization observed that achieved by the simulation results shown are acceptable.

**Keywords:** Proton exchange fuel cell (PEMFC), Creeping flow, Secondary current distribution (SIEC), Reactive flow in porous media (RFCs)

\* Corresponding author:

G. Carbajal-De la Torre, <sup>a</sup>Universidad Michoacana de San Nicolás de Hidalgo, Edificio W, Ciudad Universitaria, Francisco J. Mújica S/N C.P. 58030, Morelia Michoacán, México, (443)3223500 ext. 3148, gctorre@umich.mx.

**Ion conduction in membranes of sulfonated polyetherimide:  
A theoretical study**

**Y. A. Peña-Castañeda<sup>a</sup>; E. López-Chávez<sup>a,\*</sup>; G. González-García<sup>a</sup>,  
F. de L. Castillo-Alvarado<sup>b</sup>; J. A. Irán Díaz-Góngora<sup>c</sup>**

<sup>a</sup>Universidad Autónoma de la Ciudad de México, Fray Servando Teresa de Mier 92, 1er. Piso, Col. Centro, México, D.F., C.P. 06080, México.

<sup>b</sup>Escuela Superior de Física y Matemáticas del Instituto Politécnico Nacional Unidad Adolfo López Mateos. Col. Lindavista. Del Gustavo A. Madero. México D.F., 07738, México.

<sup>c</sup>Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Instituto Politécnico Nacional Legaria 694. Col. Irrigación. Del. Miguel Hidalgo 11500, Ciudad de México, Distrito Federal.

**ABSTRACT**

Molecular dynamics and mechanical simulations were performed to study mechanism ionic conductivity in membranes of sulfonated polyether imides with various sulfonyl groups. The method used in this study was force fields. Microscopic parameters were found and these were used to calculate the ionic conductivity in each membrane. The drive mechanism is determined and analyzed, finding that the position of the sulfonyl groups in the backbone of the polymer structure, greatly influences in the value of ionic conductivity. The model of membrane was built using polymeric chains oriented in three dimensions. The ionic species used in the simulations were hydronium and hydroxyl. The theoretical results are compared with experimental results reported in the literature. The goal of this study is to find the polymer that does the best conduction mechanism in the way to enhance the efficiency of Proton Exchange Membrane Fuel Cell (PEMFC). The ionic conductivity parameter does not necessarily have linear relationship with the number of sulfonated groups. These membranes are a proposal to supply the Nafion<sup>®</sup> membrane into PEMFC.

**Keywords:** Polyetherimide, Ion-Conduction, PEMFCs

\* Corresponding author:

Ernesto López-Chávez, +52 55 5134 9804 Ext. 11110, elopezc\_h@hotmail.com.



**Design and analysis of photovoltaic-hydrogen system for illumination and fuel cell characterization**

**J. Olmedo-González<sup>a\*</sup>; R. de G. González-Huerta<sup>a</sup>; M. Tufiño-Velázquez<sup>b</sup>; G. Contreras-Puente<sup>b</sup>**

<sup>a</sup>ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPALM, CP 07738, México, D.F.

<sup>b</sup>ESFM-IPN, Laboratorio de Física Avanzada, UPALM, CP 07738, México, D.F.

**ABSTRACT**

At the present time hydrocarbon resources are the principal source of energy. However, they have not been good for the environment and we have to consider that the demand of energy has been growing in the last decades. For this reason it is so important to develop new ways to produce energy. Renewable energy sources such as solar or wind energy are cleaner than hydrocarbons and they could satisfy the demand of energy, when the energy is administered in a correct way. One of the problems of these primary sources are their natural intermittence and hydrogen could be a good solution for this problem.

In this work is proposed a photovoltaic-hydrogen system, in the hybrid system photovoltaic modules are used to provide energy for a PEM electrolyser producing hydrogen and oxygen gases through the water electrolysis, gases produced are stored in a variable volume tanks, so they are supplied into a PEM fuel cell to generate electrical energy.

The design was developed in order to produce enough hydrogen for the two requirements, illumination or for analyses of new PEM fuel cells. It was considered the period of time for illumination and the flow rate of hydrogen and oxygen that the new PEM fuel cells could require. The analysis of the system was developed studying each part of this and developing the material and energy balance. It shows the period of time for gases production and it permits understand their efficiency and efficacy of the system. It was found that the system has a good behaviour when it is designed in order to be a flexible system, it improve the use of energy produced increasing its efficacy. Storing part is really efficient because it is not necessary auxiliary energy to store gases. However, it is suitable for small systems.

**Keywords:** Photovoltaic-hydrogen system, PEM fuel cell applications, Hydrogen Storage

\* Corresponding author:

Jorge Olmedo-González, Tel: (+52) 5527092864; e-mail: jolmedog0900@alumno.ipn.mx

**Dissociative mechanism of oxygen reduction reaction (ORR) on Pd-Cu disordered binary alloy metal surfaces: A theoretical study**

**E. López-Chávez<sup>a,\*</sup>; A. García-Quiroz<sup>a</sup>; G. González-García<sup>a</sup>; Y. A. Peña-Castañeda<sup>a</sup>;  
J. A. I. Díaz-Góngora<sup>b</sup>; F. L. Castillo-Alvarado<sup>c</sup>**

<sup>a</sup>Autonomous University of Mexico City. Av. Fray Servando Teresa de Mier 92-110. Col. Centro Histórico, Del. Cuauhtémoc, CP 06080 México, D.F.

<sup>b</sup>Research center in applied science and advanced technology of National Polytechnic Institute. Legaria 694, Col Irrigación, Miguel Hidalgo, 11500 Ciudad de México, Distrito Federal, Mexico.

<sup>c</sup>School of Physics and Mathematics of the National Polytechnic Institute. Edificio 9 de la UPALM, Zacatenco, Col. Lindavista, Gustavo A. Madero, CP. 07738, México, Distrito Federal.

**ABSTRACT**

Density functional theory (DFT) in conjunction with virtual crystal approximation is used to study the oxygen reduction reaction (ORR) as a function of the copper concentration in Pd-Cu disordered binary alloy metal surfaces. Reactivity is evaluated on the basis of an oxygen reduction reaction (ORR) dissociative mechanism of four steps, it involves the splitting of the O–O bond in O<sub>2</sub> after its adsorption, followed by hydrogenation of atomic O to OH. Then, the OH species undergoes another hydrogenation to yield H<sub>2</sub>O. For each concentration of Cu, results for low oxygen coverage are presented at zero cell potential ( $U = 0$ ), at the equilibrium potential ( $U = 1.23$  V), and at the highest potential ( $U = 0.80$  V) where all reaction steps are exothermic. The results indicate that at the ORR equilibrium potential of 1.23 V, the reactivity of all surfaces is shown to be limited by the rate of OH removal from the surface, while that at a cell potential of 0.80 V, the ORR reactivity of different surfaces is dictated by the strength of oxygen adsorption. The results are compared with other non-Pt alloys.

**Keywords:** Catalysis, Binary alloy, Oxygen reduction reaction, Dissociative mechanism

\* Corresponding author:

Ernesto López-Chávez, +52-55-51349804 ext. 11110, elopezc\_h@hotmail.com

**Numerical study of heat transfer in a PEM fuel cell with  
different flow- fields**

**J. Macedo-Valencia<sup>a</sup>; J. M. Sierra<sup>a,\*</sup>; S. Figueroa-Ramírez<sup>a</sup>; H. Mandujano<sup>a</sup>; M. Meza<sup>a</sup>**

<sup>a</sup>Facultad de Ingeniería, Universidad Autónoma del Carmen, Cd. del Carmen, Campeche C.P. 24115, México.

**ABSTRACT**

The heat generated in a proton exchange membrane fuel cell (PEMFC) may represent 50% of the total energy produced in these devices. This heat is produced mainly for three reasons: the electrochemical reactions, ohmic heating and water condensation in the fuel cell. Proper manage of these mechanisms is a critical problem to solve in the fuel cell. In this regard, a 3D numerical study of heat transfer in a PEMFC is presented in this work. The governing equations were solve using a commercial code of Computational Fluid Dynamics (CFD). Conventional and non-conventional designs of flow fields with an active area of 50 cm<sup>2</sup> were evaluated to understand two issues i) how the temperature is distributed inside the fuel cell and 2) which flow field design removes more effectively the heat from the fuel cell. Normal operating conditions of pressure and temperature were set. Dry oxygen and hydrogen were supplied to the fuel cell to avoid non desired processes as well as the appearance of liquid water on the anode side. Distributions contours of temperature, species and current density were obtained in this study. Numerical results showed that designs with multiple parallel channels dissipate more heat than conventional designs, also some non conventional designs showed better results than conventional designs. Furthermore it was found that the cathode compartment presents higher temperatures than the anode compartment. The results were validated by polarization curves and experimental data reported in the literature. From this study relevant information of heat transfer processes was obtained to improve the design of the fuel cell.

**Keywords:** Heat transfer, PEM Fuel Cell, Flow fields, CFD

\*Corresponding author:

Juan Manuel Tadeo Sierra Grajeda, Tel. : +52 777 184 35 85, E-mail adress: [juanmsg@live.com.mx](mailto:juanmsg@live.com.mx)

**Numerical evaluation of a PEM electrolyzer using  
computational fluid dynamics**

**B. A. Flores-Argáez<sup>a,\*</sup>; J. M. Sierra<sup>a,\*</sup>; S. Figueroa-Ramírez<sup>a</sup>; O. Meza-Cruz<sup>a</sup>;  
C. Patiño<sup>a</sup>**

<sup>a</sup>Facultad de Ingeniería, Universidad Autónoma del Carmen, Cd. del Carmen, Campeche C.P. 24115, México.

**ABSTRACT**

In this research a 3D computational fluid dynamics study in a proton exchange membrane electrolyzer is presented. The aim of this work was to model the transport phenomena that take place inside the electrolyzer, such as species distributions, and temperature variations in the electrodes. The governing equations of continuity, momentum, energy, species transport, and the Butler-Volmer model for the electrochemical reactions were solved using a commercial code. The operating conditions set in the model were 2 atm and 75 °C, for pressure and temperature, respectively. Two flow field designs were simulated in a single model of electrolyzer. Both designs are constituted by a membrane, electrodes and monopolar plates. Contours of pressure, mass fraction, temperature, current density and ionic conductivity were obtained by numerical simulation. These results showed that the distribution of pressure, velocity and temperature are not uniform across the active area, these parameters vary from the inlet to the outlet and they are directly related to the design of the channels. Likewise, results demonstrated that electrolyzer performance is sensitive to reactants flow rate, therefore is absolutely necessary that the electrodes receive the same amount of water. Accumulation of gas and hot spots in non desired areas will be avoided when water distribution is homogeneous. Numerical polarization curves were obtained and validated by experimental data reported in the literature. In this study, it was possible to obtain relevant information on the mass transport, heat transfer and electrochemical reactions that take place in the PEM electrolyzer. These results can be used as criteria to improve the design and performance of the PEM electrolyzer.

**Keywords:** PEM electrolyzer, Flow field, CFD

\*Corresponding author:

Juan Manuel Tadeo Sierra Grajeda, Tel. : +52 777 184 35 85, E-mail adress: juanmsg@live.com.mx

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Design and characterization of fuel cell regenerative for social communications**

**H. Martinez-Espinoza<sup>a</sup>; B.Escobar<sup>b</sup>; R.Barbosa<sup>c</sup>; G. Rodriguez-May<sup>a</sup>;  
V. M. Sanchez<sup>c</sup>; J. C. Cruz<sup>a\*</sup>**

<sup>a</sup>Instituto Tecnológico de Chetumal, Av. Insurgentes s/n, Chetumal, Quintana Roo 77013, México

<sup>b</sup>Centro de Investigación Científica de Yucatán, A.C., Calle 43 No. 130 Colonia Chuburná de Hidalgo, Mérida, Yucatán 97200, México

<sup>c</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Quintana Roo 77019, México

**ABSTRACT**

The Unitized Regenerative Fuel Cell (URFC) is a system that works like a secondary battery. These function as a Proton Exchange Membrane fuel cell (PEMFC) and water electrolysis PEM (WEPEN). The oxygen reduction reactions (ORR) in a PEMFC cathode and oxygen evolution reaction (OER) at the anode of a WEPEN are limitations to these reactions in the system. Each part has its timing; first, the gas production takes place, after obtaining both gases, the combination of oxygen and hydrogen takes place to produce electricity. The information describes the design and electrochemical characterization employed in this concept. The material used in the Oxygen compartment was Pt – IrO<sub>2</sub> while in the Hydrogen compartment, Pd/C was used. The technique to introduce the materials was by hot spray, the amount of Pt – IrO<sub>2</sub> (50:50 wt. %) catalyst was 1 mg · cm<sup>2</sup> and for the Pd/C (30% wt. Pt) which acts as dual hydrogen electrode, for this material a portion of 0.5mg · cm<sup>2</sup> was introduced. The electrochemical parameters were determined using the techniques of linear voltammetry, electrochemical impedance spectroscopy, chronoamperometry and chronopotentiometry. It was determined the amount of hydrogen production at 27 ° C at different conditions; it was obtained the maximum power in both modes. A Unitized Regenerative Fuel Cell for science in schools and higher secondary education was obtained.

**Keywords:** URFC, Catalyst , Water electrolysis

\* Corresponding author:

Dr. Julio Cesar Cruz Arguello, +9831043002, Mexico,jcruz@itchetumal.edu.mx



**Modelling membraneless fuel cell with finite element method**

**M. González-Vázquez<sup>a,\*</sup>; L. H. Juárez-Valencia<sup>a</sup>**

<sup>a</sup>Universidad Autónoma Metropolitana, Unidad Iztapalapa, San Rafael Atlixco No. 186, Col. Vicentina, Iztapalapa, 09340, México

**ABSTRACT**

Fuel cells are devices that generate electricity, one class of fuel cell are so called membraneless fuel cells where the separation of the reactants, the fuel and oxidant, are made by stable laminar flows. The mathematical model for a membraneless fuel cell is built up from the Poisson-Nernst-Planck (PNP) equations allowing for diffuse charge in solution with a transport term linked to the solution of the the Navier-Stokes (NS) equations.

The applications of the Navier-Stokes-Poisson-Nernst-Planck (NS-PNP) equations go of classic chemical and electrochemistry engineering, until technologies of the environment as desalination and alternative power, as well as biotechnology, biomedical engineering and micro-electro-mechanical systems, among others. From a mathematical point of view, is very difficult to derive analytical solutions of the NS-PNP equations, even for the steady-state system with a very simple geometry. The main difficulty arises from the nonlinear coupling of the velocity, the electrostatic potential and the concentrations of ions. On the other hand, the cost of developing experiments is high. Thus it, is necessary to development numerical methods for the solution of the NS-PNP equations.

In this communication the numerical solutions of the NS-PNP equations for some cases of membraneless fuel cells in two dimensions will be presented. These numerical solutions were obtained from an iterative algorithm using the operator-splitting, projection method and finite element method.

**Keywords:** Membraneless fuel cell, Navier-Stokes-Poisson-Nernst-Planck equations, Finite Element, Microchannel

\* Corresponding author:

Miguel González-Vázquez, Tel: (+52) (01) 55 5804 4654, Fax: (+52) (01) 55 5804 4653, migonzalezv@xanum.uam.mx

**APQP methodology applied in the design and manufacture of  
alkaline electrolyser**

**M. Horcasitas-Verdiguél<sup>a,\*</sup>; R. G. Gonzalez-Huerta<sup>b</sup>; J. M. Sandoval Pineda<sup>a</sup>**

<sup>a</sup>ESIME-IPN UA, Sección de posgrado, Av. de las Granjas 682, C.P. 02250, México, D.F.

<sup>b</sup>ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPALM, 07738, México D.F.

\*Mail: hove\_lenuma@hotmail.com

**ABSTRACT**

This communication analyzes the main main problems of the alkaline electrolysis, i.e., the process of manufacturing, geometry and materials, its requirements for a design that allows control parameters such as electric current, gas outlet, optimal level of electrolyte, corrosion, sealing system, etc., this with an objective, manufacture and get to get an electrolyzer with maximum efficiency. Therefore the use of Hydrogen produced from electrolysis of water may be used as an additive with fossil fuels for transport that can reduce certain parameters such as CO and CO<sub>2</sub> pollutants., And its overall objective to reduce automotive emissions.

Hydrogen is of particular interest as secondary energy carrier because it has the potential to be generated in situ, stored and transported. Due to the particular application allows Oxyhydrogen gas generation in situ and is not be high purity, as this gas will be injected into internal combustion engines as an additive to the mixture air-fuel (gasoline or diesel).

This paper focuses on the APQP methodology for the design of an alkaline electrolyzer. APQP is an analytical methodology used to ensure potential problems are considered and addressed through the process of product development and process (APQP -Planning advanced quality of a product). With gas generation technology Oxyhydrogen by alkaline electrolysis, the Methodology application and appropriate manufacturing It's possible to obtain reached to develop a more efficient reactor in all its features and a better design with optimal materials and special components.

Good design and manufacture of the components of the electrolyzer substantially improve the performance thereof, as well as the efficiency current and voltage as a good internal connection between each electrode decreases overpotential and the distance between anode and cathode reduce the resistance.

**Keywords:** Hydrogen, APQP, Alkaline electrolysis, Manufacturing

\* Corresponding author:

M. Horcasitas-Verdiguél, ESIME-IPN UA, Sección de posgrado, Av. de las Granjas 682, C.P. 02250, México, D.F., E-mail: hove\_lenuma@hotmail.com



**Thermodynamic analysis of the autothermal partial oxidation/steam reforming of ethanol by MeO (Me = Ni, Cu) with CO<sub>2</sub> capture**

**V. Collins-Martínez; M. J. Meléndez-Zaragoza; A. López-Ortiz\***

Departamento de Ingeniería y Química de Materiales, Centro de Investigación en Materiales Avanzados, S.C., Miguel de Cervantes 120, Chihuahua, Chih., México, 31136, México.

**ABSTRACT**

Hydrogen is generally considered as a clean and high efficient energy carrier that can be employed for power generation through fuel cell units, with innocuous water as the only by-product, to decrease the release of pollutants into the atmosphere. Today, there is a developing interest for hydrogen generation from renewable sources such as bio-oil, bio-gas, bio-ethanol or bio-butanol etc. Among the different renewable feedstock options, ethanol has been viewed as an appealing feedstock because of its relatively high hydrogen content, accessibility, nontoxicity, ease of handling and safety. The present thermodynamic analysis is aimed to explore autothermal conditions at equilibrium for a high H<sub>2</sub>-syngas production under the combined ethanol steam reforming (SRE), chemical looping partial oxidation (CLPOX) and CO<sub>2</sub> solid absorption reaction system. SRE studied conditions were H<sub>2</sub>O/C<sub>2</sub>H<sub>6</sub>O = 3-6 molar ratio, CLPOX employed NiO or CuO as metal oxide (MeO) oxygen carriers from MeO/C<sub>2</sub>H<sub>6</sub>O = 0.05-1.5 molar ratio, while 2 kmols of CaO were used for CO<sub>2</sub> capture in a T range of 100-900 °C at 1 atm. NiO most favorable adiabatic conditions (T ≥ 500 °C and C ≤ 0.1 kmols) were: H<sub>2</sub>O/C<sub>2</sub>H<sub>6</sub>O = 3 and NiO/C<sub>2</sub>H<sub>6</sub>O = 0.05-0.5. While, for CuO was at H<sub>2</sub>O/C<sub>2</sub>H<sub>6</sub>O = 4, CuO/C<sub>2</sub>H<sub>6</sub>O = 0.5 and T<sub>adiab</sub> = 529 °C. These favorable reaction conditions are the product of the combination of the exothermic carbonation reaction and its influence over the thermodynamic equilibrium over the POX and SRE endothermic reactions.

**Keywords:** Combined SRE CLPOX and CO<sub>2</sub> capture, Autothermal thermodynamic conditions

\* Corresponding author:

Dr. Alejandro López-Ortiz, Tel: +052 614 4394815, E-mail: alejandro.lopez@cimav.edu.mx

**DFT study of  $W_{1-x}Mo_xO_3 \cdot 0.33H_2O$  ( $x=0$  to 1) photocatalyst:  
importance of +U and +J on-site terms**

**J. Camarillo-Cisneros\*; A. Arzola-Rubio**

Centro de Investigación en Materiales Avanzados S. C., Miguel de Cervantes 120, C. P. 31136, Chihuahua, Chih. México

**ABSTRACT**

Hydrogen production is a technological challenge for a future energy supply, due to required efficient and stable systems, such as water splitting, photocatalysis and solar energy. Water splitting activated by solar light is a very important goal in this issue.  $W_{1-x}Mo_xO_3$  based semiconductors are promising systems for hydrogen production via photocatalysis. However, most of these results come from experimental tests with a lack of theoretical models to accurately describe the chemical phenomena taking place between the phase interactions. In this work, these Density Functional Theory (DFT) calculations using the framework of Hubbard model; DFT+U additionally with the on-site exchange contribution term J. Both U and J terms are systematically mapped to define a realistic model from bulk to the surface oxides. These results represent an important first step towards a general description of experimental measurements performed by us on  $W_{1-x}Mo_xO_3 \cdot 0.33H_2O$  ( $x=0$  to 1) photocatalytic particles.

**Keywords:** DFT, +U and +J on-site,  $W_{1-x}Mo_xO_3$  photocatalyst

\* Corresponding author:

Javier Camarillo Cisneros, phone: +526144391129; e-mail: javier.camarillo@cimav.edu.mx

**Synthesis, characterization and photocatalytic evaluation of  
 $M_{1-x}M'_xWO_4$  ( $M, M' = Ni, Co, Cu$  and  $Mn$ ) Tungstates**

**X. A. López<sup>1,2</sup>; A. F. Fuentes<sup>2</sup>; M. Meléndez Zaragoza<sup>3</sup>;  
J. A. Díaz Guillén<sup>1</sup>; A. Lopez Ortiz<sup>3</sup>; V. Collins-Martínez<sup>3\*</sup>**

<sup>1</sup>Instituto Tecnológico de Saltillo, Blvd. V. Carranza No. 2400, Col. Tecnológico Saltillo, C. P. 25280 Coahuila, México

<sup>2</sup>CINVESTAV del IPN, Unidad Saltillo, C.P. 25900, Ramos Arizpe, Coahuila México

<sup>3</sup>Centro de Investigación en Materiales Avanzados S. C., Miguel de Cervantes 120, C. P. 31136, Chihuahua, Chih. México

**ABSTRACT**

Photocatalysis is a technology that can be applied to solve environmental and energy problems such as the production of hydrogen from the dissociation of the water molecule. Tungstates exhibit many potential applications in different areas of technology due to their excellent electrical properties. Nanostructured tungstate materials are known for their wide applications in conventional catalysis, as scintillator material, in photoluminescence, optical fibres and as materials in microwave technology. Even though these present enough chemical and thermal stability, very scarce reports are found in the literature related to their uses as photocatalysts for hydrogen production through water splitting. The aim of the present study is the synthesis and characterization of family tungstate  $MWO_4$  ( $M = Co, Cu, Mn$  and  $Ni$ ) materials through co-precipitation in order to evaluate their photocatalytic activity towards the production of hydrogen within the visible light range. Characterization consisted in XRD, BET, UV-Vis and SEM, while the photocatalytic evaluation was as follows: 200 mg of  $CuWO_4$ ,  $CoWO_4$ ,  $MnWO_4$  and  $NiWO_4$  powders were individually suspended in water and methanol, the latter used as a sacrificial agent. The water suspension was placed inside a sealed quartz batch photoreactor under constant stirring and illuminated by a 250 W mercury lamp for 8 h with gas evolution being monitored by gas chromatography (GC). Preliminary results indicate that the employed synthesis method was effective to obtain the required crystalline phase. However, optimal conditions are needed to decrease particle size and increase the tungstates surface areas. The bandgap energy of these tungstates was found to be within the visible light spectrum with a variation between 2.24 eV for  $CoWO_4$  to 2.56 eV for  $MnWO_4$ , respectively. Maximum hydrogen production was achieved by sample  $MnWO_4$  with  $139 \mu\text{mH}_2/\text{g}_{\text{cat}}$ , while the lowest production was observed for sample  $CoWO_4$  with  $24 \mu\text{mH}_2/\text{g}_{\text{cat}}$ . From these preliminary results it can be inferred that simple and mixed metal transition tungstates can be considered as potential candidates, as photocatalysts for  $H_2$  production via the splitting of the water molecule under visible light irradiation.

**Keywords:**  $H_2$  generation, Water splitting, Photocatalysis, Tungstates

\* Corresponding author:

Virginia Collins Martinez, phone: +526144391129; e-mail: virginia.collins@cimav.edu.mx



## **Renewable energy systems**



**Hydrodeoxygenation of oxygenated organic compounds using Ni /  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> performed by the wet impregnation incipient method**

**B. N. López-García<sup>a,\*</sup>; M. Sánchez-Cárdenas<sup>a</sup>; J. Medina-Valtierra<sup>b</sup>**

<sup>a</sup>Universidad Politécnica de Aguascalientes, Calle Paseo , San Gerardo, 207, Aguascalientes, Ags., México, 20342.

<sup>b</sup>Instituto Tecnológico de Aguascalientes, Av. Adolfo López Mateos Ote. No. 1801, Fracc. Bona Gens, Aguascalientes, Ags., México, 20256

**ABSTRACT**

A supported Nickel catalyst on gamma alumina and performed by the wet impregnation incipient method was tested for the hydrodeoxygenation of oleic acid which is considered as a model molecule of oxygenated organic compounds. The catalyst was performed by a physical method of Bohemia and a solution of Nickel (II) tetrahydrate acetate until a homogeneous paste which was left to be dried at a current temperature. After drying the paste, it was performed a process of extrusion to obtain tablets of the same size. Finally the tables were calcined at 510 ° C in oxygen to obtain at the end nickel oxide deposited on gamma alumina. The reduction of the catalyst in the reactor was performed by applying a flow of hydrogen at 400 ° C, whereby Ni /  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> was obtained.

The experiments of hydrotreating were performed in a tubular reactor of stainless steel by using batches at 320 ° C, 20 bar H<sub>2</sub> pressure, 200 rpm and 5 hours of reaction. Data conversion of oleic acid and yields alkanes n-C<sub>17</sub> and n-C<sub>18</sub> were calculated from GC.

By analyzing the products of oleic acid hydrotreating using a catalyst with 3% in weight of Ni, it was obtained a percent conversion of oleic acid of 55.3% and a yield molar total n-C<sub>17</sub> + n-C<sub>18</sub> of 48.7%. By performing an analysis of the amount of n-alkanes even and odd generated in the reaction, it was obtained a relationship of (decarboxylation + decarbonylation)/hydrodeoxygenation of 1.59. This process indicates that Nickel is an appropriate active phase to accelerate and direct the actions of hydrodeoxygenation as well as to obtain alkanes n-C<sub>18</sub> considering that the overall reaction remains a slight domain to the decarboxylation + decarbonylation reactions for this catalyst.

**Keywords:**Hydrodeoxygenation, Decarboxylation, Decarbonylation, Oleic Acid

\* Corresponding author:

López García Brenda Nayeli,(0449)-449-187-98-29, up120083@alumnos.upa.edu.mx

**Energy balance analysis of a solar-hydrogen hybrid system integrated to a sustainable house**

**A. Yunez Cano<sup>a</sup>; R. de G. González Huerta<sup>b</sup>; R. Barbosa Pool<sup>c</sup>;  
M. Tufiño Velázquez<sup>d\*</sup>; B. Escobar<sup>e</sup>**

<sup>a</sup>CIITEC-IPN, Cda. Cecati s/n, Col. Sta. Catarina, CP 02250 Azc., México D.F.

<sup>b</sup>ESIQIE-IPN, Lab. Electroquímica y Corrosión, UPALM, CP 07738, México, D.F.

<sup>c</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal 77019, Q. Roo, México

<sup>d</sup>ESFM-IPN, Laboratorio de Física Avanzada, UPALM, CP 07738, México, D.F.

<sup>e</sup>CICY, A.C., Calle 43 No.130 Col. Chuburná de Hidalgo, Mérida, Yucatán 97200, México.

**ABSTRACT**

One of the most interesting developments of energy systems based on the utilization of hydrogen is their integration with renewable sources of energy. In fact, hydrogen can operate as a storage and carrier of the energy produced by these primary sources. The design and operation of the system change noticeably depending on the type and availability of the primary source. In this paper, we describe the performance of a stand-alone energy system that uses solar energy as the primary source, which comprises PV solar panels, an electrolyzer, a hydrides storage tank and a proton exchange membrane fuel cell (PEMFC). The sizing and design of these technologies need to meet the local microclimate in order to reach high efficacies. An analytical model to size, analyze and assess the performance of a hybrid photovoltaic/hydrogen (PV/H<sub>2</sub>) energy conversion system using real weather data is presented in this work. The analysis includes an energy balance and a description of the behavior of electrical variables of the system components; the subsystems efficacy is calculated and from the obtained results, improvements to increase the efficiency by the use of surplus energy produced by the hybrid system are proposed. We used solar radiation measurements from a meteorological monitoring station placed on the roof of the sustainable house located in the north side of Mexico City. PV solar panels supply the electric power to satisfy the electric load. Surplus energy is delivered to an electrolyzer to produce the hydrogen to be stored in a hydrides tank. In energy deficit hours a PEMFC covers partially the electric demand; therefore the hybrid system efficacy is calculated based on the level of energy stored and the fulfillment of the electric load.

The authors thank CONACYT: Programa de Redes Temáticas (RTH2) Projects 252003 and 249795; and IPN-SIP Multidisciplinary Projects 1683 and 1725.

**Keywords:** Energy balance analysis, Solar-hydrogen hybrid system, Sustainable house

\* Corresponding author:

Miguel Tufiño Velázquez, (+52) 55 57296000 ext.46138, mitufinovel@gmail.com

**Reactor with agitation of double twist for hydrotreating of oxygenated organic compounds**

**S. L. Zamorano-Murillo<sup>a,\*</sup>; M. Sánchez-Cárdenas<sup>a</sup>; J. Medina-Valtierra<sup>b</sup>**  
**R. A. Ortiz-Medina<sup>a</sup>; Z.J. Pineda-Hernández<sup>a</sup>**

<sup>a</sup> Universidad Politécnica de Aguascalientes, Calle Paseo , San Gerardo, 207, Aguascalientes, Ags., México, 20342.

<sup>b</sup> Instituto Tecnológico de Aguascalientes, Av. Adolfo López Mateos Ote. No. 1801, Fracc. Bona Gens, Aguascalientes, Ags., México, 20256

**ABSTRACT**

A stainless steel reactor for hydrotreating of waste oils and their conversion to biodiesel has been designed and build. The reactor can run by batches or continuous flow. It has the capacity to convert 100 mL of waste oil at temperatures exceeding 400 degrees Celsius and at H<sub>2</sub> pressures of up to 20 MPa. The stainless steel cylindrical reactor is introduced to a jacket containing a heating tape connected to a temperature controller. In the inside of the reactor there is a mechanism consisting of a roller bearing that was placed at the top, that intended to facilitate the rotation and bring stability in the assembly of the reactor with the heating jacket. At the bottom of the reactor, there are agitation blades that gives homogeneity to the agitation of the mixture. On the outside, the reactor has a turmoil mechanism where is connected with a shaft and assembled to an engine. The engine controls speed and rotation, and allows agitation with full and half turns of the shaft.

To ensure good performance and safety of operation, a simulation study was carried out in order to determine the vulnerabilities of the reactor in critical or nominal working conditions. It takes into account the strength of the material and its possible deformation for such conditions. The study simulates the loads and pressures that the reactor will be subject to and determinates the way that the material will answer, taking into account the geometry of the whole reactor. The pressure is estimated to be at 40 KPa as a maximum allowed for this reactor, whereas the pressure of work for the hydrotreating processes is well below this limit, which is acceptable to the established range. Studies of Von Mises stress applied to the structure of the simulated solid are located below the elastic limit of the material, so the structure of the reactor remains stable and safe. Tests were carried out to the hidredeoxygenation of the oleic acid using Pt and Ni catalyst supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

In the experiments, it was observed that the catalyst with 2% by weigh of Pt presented a (descarbonylation + decarboxylation) / Hydrogenation ratio of 18.2, which in comparison with the 2% by weight Ni catalyst with a 1.23 ratio shows that the Pt catalyst has a bigger acceleration reaction for descarbonylation and decarboxylation.

**Keywords:** Hydrotreating, Reactor, Agitation

\*Corresponding author: Zamorano Murillo Saira Lizette, (0449)-449-142-39-48  
up130248@alumnos.upa.edu.mx





## **Improvement of novel microbial fuel cell design for wastewater treatment**

**A. Rodrigo M. Ochoa<sup>a</sup>; K. Sathish-Kumar<sup>a\*</sup>; O. Solorza-Feria<sup>b</sup>; J. Tapia-Ramírez<sup>c</sup>**

<sup>a</sup>Universidad Politécnica de Aguascalientes, Ingeniería en Energía Calle Paseo San Gerardo No. 207. Fracc. San Gerardo. Aguascalientes, Ags. México, 20342.

<sup>b</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Química, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. 07360.

<sup>c</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Genéticas y Biología Molecular

### **ABSTRACT**

In our previous report, we proposed the novel microbial fuel cells (MFCs) design from pencil (SMH2014). Further more, we known the 6M sulfuric acid treated pencil based integrated MFCs exhibit better performance. At the continues of that point, we have tried to improve the performance of pencil based intergrated MFCs by increasing the anodic current collector surface area. In pencil, the graphite rod could act as anode besides submerged with wooden portion into the raw high concentrated wastewater solution, and remained wooden portion bound with Pt/Carbon cloth (Cathode) exposed to air. Raw high concentrated waste waters was used both as inoculum to form electrochemically active bacteria on graphite based anode and also as the medium to be treated. Later we applied the graphite felt on the anodic current collector (graphite rod) of pencil based integrated MFCs.

The highest maximum power density ( $191.6 \text{ mW/m}^3$ ) is obtained in graphite felt anode, which is 65.49 % higher than that of graphite rod as anode ( $66.1 \text{ mW/m}^3$ ) in pencil based integrated MFCs. The large surface area properties of the graphite felt anode play a rather important role in anodic reaction. Batch operation of graphite felt anode showed the average power density  $1.52 \text{ mW/m}^3$ , which is 54.38% higher than that of graphite rod as anode  $0.83 \text{ mW/m}^3$ . The average COD removal efficiencies were 91.77% and 82.65 % in the graphite felt anode and graphite anode, respectively. Further, we powered the 3 digital clock by 3 serially connected graphite felt anode as MFCs, which exhibited the average power density  $10.3 \text{ mW/m}^3$  and potential 1.1487 V. These results show graphite felt is suitable for pencil based integrated MFCs as anode could increase the extracellular electron transfer in that way increase power production in MFCs.

**Keywords:** Microbial fuel cells, Graphite felt, pencil, Air cathode

\* Corresponding author: Kamaraj Sathish-Kumar, +01 (449) 442 1400 ext: sathish.bot@gmail.com, sathish-kumar.kamaraj@upa.edu.mx

**Use of Clay tube as integrated Microbial fuel cell for wastewater treatment**

**A. de J. Robledo Ruiz<sup>a</sup>; K. Sathish-Kumar<sup>a,\*</sup>; O. Solorza-Feria<sup>b</sup>;  
J. Tapia-Ramírez<sup>c</sup>**

<sup>a</sup>Universidad Politécnica de Aguascalientes, Ingeniería en Energía Calle Paseo San Gerardo No. 207. Fracc. San Gerardo. Aguascalientes, Ags. México, 20342.

<sup>b</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Química, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. 07360.

<sup>c</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Genéticas y Biología Molecular

**ABSTRACT**

Simplified Microbial fuel cells (MFCs) design attracts the attention of researcher, in order to scale up the process. In this context, we have proposed the simplified MFCs design from clay tube based integrated MFCs, which utilizes the real wastewater collected from the polytechnic university of Aguascalientes served as waste to be treated as well as biocatalyst. Clay materials are commonly phyllosilicates or layer silicates. Its cation exchange capabilities, low permeability, and long term structural stability triggers the interest. Moreover, partially submerged clay tube into the water would arise on the lateral direction through capillary force. We could exploit this process along with proton hopping facilitate the proton mobility towards vertical direction on the clay tube. Remarkably, we could optimize the level of submerged clay tube into wastewater. Since we performed the two kinds of experiments. First, we could submerged the 2 part of clay tube into the wastewater and 1 part of the clay tube exposed to the air (2:1 ratio). Later experiment, we performed the submerged 3 part of the clay tube and 2 part of clay exposed to air (3:2). From that 3: 2 ratio integrated clay tube MFCs exhibited highest power density  $17.54 \text{ mW/m}^3$ , current density  $55.97 \text{ mA/m}^3$  at  $0.313 \text{ V}$  potential. Moreover, it exhibit the highest COD removal of 91 %. Further, we connected the three 3:2 ratio integrated clay tube MFCs in series and powered the Digital Clock. Hence, Our simplified MFCs design could possible scale up the process and more importantly without using any additional input energy (purging, agitation, temperature, circulation and etc...) [Patent Pending].

**Keywords:** Clay, Proton transfer, Wastewater, Proton hopping

\* Corresponding author: Kamaraj Sathish-Kumar, +01 (449) 442 1400 ext: sathish.bot@gmail.com, sathish-kumar.kamaraj@upa.edu.mx

**Instant disposable microbial-battery from paper cup for electronic applications**

**M. C. Vega Reyes<sup>a</sup>; A. Rodrigo M. Ochoa<sup>a</sup>; K. Sathish-Kumar<sup>a,\*</sup>;  
O. Solorza-Feria<sup>b</sup>; J. Tapia-Ramírez<sup>c</sup>**

<sup>a</sup>Universidad Politécnica de Aguascalientes, Ingeniería en Energía Calle Paseo San Gerardo No. 207. Fracc. San Gerardo. Aguascalientes, Ags. México, 20342.

<sup>b</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Química, Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. 07360.

<sup>c</sup>Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Departamento de Genéticas y Biología Molecular

**ABSTRACT**

Herein, we present a paper cup based integrated microbial fuel cell (PC-MFC) for instant power production. We placed the graphite felt electrode to the inside of the paper cup that act as a anode. Raw high concentrated wastewaters collected from the Polytechnic University of Aguascalientes was used both as inoculum to form electrochemically active bacteria and the medium to be treated. These wastewater poured into paper cup. Outer portion of the paper cup was tied with Pt/Carbon cloth exposed to air as cathode. This MFC exhibited the maximum power density  $18.15 \pm 5.19 \text{ mW/m}^3$  and current density  $82.64 \pm 48.60 \text{ mA/m}^3$  at 0.22 V. Further, we serially connected the two instant PC-MFCs to power the digital clock. This serially connected MFCs were showed the average volumetric power density of  $318.75 \pm 149.7 \text{ mW/m}^3$  at  $1.164 \pm 0.21 \text{ V}$  during the 550 hrs of operation. Individual PC-MFC-1 and PC-MFC-2 were revealed the average volumetric power density of  $0.460 \pm 0.14 \text{ mW/m}^3$  and  $0.513 \pm 0.31 \text{ mW/m}^3$  respectively. Moreover, PC-MFC-1 and PC-MFC-2 exhibit the COD removal of 33.66 % and 33.84 %. This PC-MFCs has the advantages of ease of use for the small electronics applications and high portability (Patent pending).

**Keywords:** Bio-battery, paper cup, Wastewater, Graphite felt

\* Corresponding author: Kamaraj Sathish-Kumar, +01 (449) 442 1400 ext: sathish.bot@gmail.com, sathish-kumar.kamaraj@upa.edu.mx

**Electrochemical properties of low cost free-metal electrocatalyst obtained from waste materials**

**E. Montes-Bocanegra<sup>b</sup>; C.M López-Badillo<sup>b</sup>; D. Lardizabal-Gutierrez<sup>c</sup>;  
M. Figueroa-Chavez<sup>d</sup>; F.J. Rodríguez Varela<sup>a</sup> and I. Alonso-Lemus<sup>a\*</sup>**

<sup>a</sup>Centro de Investigación y Estudios Avanzados del Instituto Politecnico Nacional Unidad Saltillo, C.P. 25900, Ramos Arizpe, Coah., México.

<sup>b</sup>Facultad de Ciencias Químicas, Universidad Autónoma de Coahuila, Blvd. V. Carranza y José Cárdenas Valdés, C.P. 25280, Saltillo, Coah., México.

<sup>c</sup>Laboratorio de Energía y Medio Ambiente. Instituto Tecnológico de Cancún. Av. Kabah km. 3S/N. Cancún, Quintana Roo, México.

<sup>d</sup>Facultad de Ingeniería Civil, Universidad Autónoma de Nuevo León, , Av. Universidad s/n, Ciudad Universitaria, San Nicolás de los Garza, Nuevo León C.P. 66451, Mexico

**ABSTRACT**

In this work, the synthesis of novel electrocatalysts obtained from leather scraps is reported. Using simple thermochemical treatments, a waste material was using as raw material in order to acquire properties that make it a promising material in electrocatalysts for fuel cells. First the leather was pyrolyzed in N<sub>2</sub> atmosphere (700-1000°C). After, the pyrolyzed samples were doped by hidrothermal treatment at 180°C during 24 hours. Finally, each catalyst were washed and dried. Structural features of electrocatalysts from leather were characterized by Raman spectroscopy and X-Ray difraction powder. The morphology was determinate by scanning electron microscopy (SEM). The activity for oxygen reduction reaction (ORR), was evaluated by rotary disk electrode technique (RDE), the results indicate that electrocatalytic activity of this electrocatalyst is high compared with commercial electrocatalyst (20% Pt / C), one of the materials denotes higher current density and on-set potential very close to Pt/C evaluated at the same conditions.

**Keywords:** Hydrogen production, Nanomaterials, Hydrogen economy

\* Corresponding author:

Ivonne L. Alonso Lemus, CATEDRA CONACyT, + 52 01 (844) 4389626, ivalemus@gmail.com

**Oxyhydrogen gas production for fuel enriched in  
internal combustion engine**

**J.A. Fuentes Coutiño<sup>a,b,\*</sup>; J.M. Pineda Sandoval<sup>a</sup>; R.G. González-Huerta<sup>b</sup>**

<sup>a</sup>IPN-ESIME-Azc, SEPI, Av. De las Granjas, N°.682, Azcapotzalco. CP. 02250. México DF.

<sup>b</sup>ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPLAM, CP 07738, México, D.F

**ABSTRACT**

The limited fossil fuel reserves and severe environmental pollution have pushed studies on fuel economy in internal combustion engines (ICE). This paper investigated the effect of hydrogen and oxygen blends (oxyhydrogen gas) addition on the performance of gasoline engine. In this proposal, an alkaline electrolyzer prototype was designed and constructed for oxyhydrogen production to enrich gasoline used in an ICE. There are two alkaline electrolysis cell configurations, namely, the monopolar and the bipolar. From the manufacturing point of view, the monopolar configuration is simple and easy to fabricate and maintain but suffers from high electrical currents at low voltages, causing large ohmic losses. The bipolar configuration reduces the ohmic losses on the electrical circuit connectors but demands much greater precision in design and manufacturing to prevent the electrolyte and gas leakage between cells. Methodologies and manufacturing processes are analyzed, prototype development is detailed, including material selection, handling and security, manufacturing process and efficiency. In this work, we use monopolar configuration, regarding it product could be marketed in the short term.

The test was performed on a modified CIE (a piston to 125 cc) equipped with an oxyhydrogen gas injection system. The engine was run at a typical city-driving speed of 1000 and 2000 rpm with various excess air ratios and five standard oxyhydrogen volume fractions in the total intake gas of 0%, 5%, 10%, 15% and 20%, it was done an analysis about reduce gasoline consumption. The engine performance, service life and reducing the use of gasoline are analyzed, a perspective of the pollutants reduction and environmentally damaging emissions is done. Security measures at every stage are considered. 5% oxyhydrogen enriched, produce around 10% less gasoline consumption and a reduction of greenhouse gases such as carbon monoxide (CO) and carbon dioxide is also reduced in 5% to 10% approximately.

**Keywords:** Alkaline Electrolyzer, Oxyhydrogen gas, Internal combustion engines, Saving gasoline

\*Jesus Adrian Fuentes Coutiño; (55)5533876682; E-mail: j\_fuentesc@hotmail.com

**Simulation process of alkaline electrolyzers to save natural gas in food dehydration plant**

**J.A. Gutiérrez Rodríguez<sup>1,2,\*</sup>; S.A. Romo Ríos<sup>1,2</sup>; R. de G. González Huerta<sup>2</sup>**

<sup>1</sup>UNAM-Facultad de Química, C. Universitaria, Circuito Exterior S/N, CP 04510, México D.F.

<sup>2</sup>IPN-ESIQIE, Lab. Electroquímica y Corrosión, UPALM, CP 07738, México D.F.

**ABSTRACT**

Nowadays, world starts to live the decrease of oil production. This is reflected on the constant costs increase in hydrocarbon products. For instance the liquefied gas in México shown a 20% of increase in its cost in only three years (2012-2015). Therefore, it is necessary to search for alternative energies that can be useful in the existing infrastructure and also work independent from the conventional energies. Hydrogen has been recognized as the most promising future energy carrier. At present, industrial hydrogen production processes are not independent of traditional energy resources, which could easily cause secondary pollution. Mexico has abundant solar energy resources and the installed capacity of solar power (photovoltaics system-PV) grows every year.

In this paper, solar power is used in water-electrolytic process, which will contribute to the development of green economy and low carbon economy in Mexico. We produce oxyhydrogen gas (oxygen and hydrogen mix) obtained from alkaline electrolysis in order to save natural gas in food dehydration plant. The sizing of a hybrid system (solar-hydrogen) has to consider the steady state characteristics, unsteady profiles of the site energy source and the electricity loading demand. Although these profiles restrict the power of the subsystems to a limited range of possibilities, the numbers of possible combinations are numerous. So first, small alkaline electrolyzers prototypes were designed, performance (voltage vs current curves) and oxyhydrogen gas production were obtained. Second, this allows design bigger electrolyzer for enrichment of hydrocarbon lines in industrial processes which spend much energy. Finally, a simulation process was developed to integrate a hybrid system (PV-alkaline electrolyzer) with a food dehydration plant. Authors thank CONACYT to the Programa de Redes Temáticas (RTH2) projects 252003 and 249795; and IPN SIP multidisciplinary project 1683.

**Keywords:** Hydrogen production, Hydrogen applications, Alkaline electrolysis, Save fossil fuel

\* Corresponding author:

Juan Antonio Gutiérrez Rodríguez, +52-1(55) 284 72 617, j.antonio92@gmail.com



**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Evaluation a stand-alone hybrid system PV-WT-FC and batteries in Mexico**

**A.M. Martínez-Bañuelos<sup>a</sup>; J. C. Jaime-Dominguez<sup>a</sup>; J. R. Espinoza-Lumbreras<sup>a</sup>;  
S. M. Durón-Torres<sup>a</sup>; C. Guzmán<sup>b</sup>**

<sup>a</sup>UACQ–UAZ, CU Siglo XXI Edificio 6, Km 6 Carr. Zac–Gdl, La Escondida Zacatecas, Zac, C.P. 96160, México.

<sup>b</sup>Facultad de Ingeniería, Universidad Autónoma de Querétaro, Cerro de las Campanas, C.P. 76000, Santiago de Querétaro, Qro., México.

**ABSTRACT**

The use of renewable energy sources such as solar radiation in photovoltaic (PV) and wind speed wind turbine (WT) to provide the energy demand in isolated places has been possible due to their use altogether, this type of system is known as hybrid power system. However one of the main problems with the isolated hybrid power systems is its intermittency due to fluctuating weather condition, For this reason sought different energy systems that can help power generation to achieve also have a stable power generation is very important.

For that reason the objective of this work was the use of fuel cells (FC) as a secondary power generation system, it is performed to compare a PV hybrid system of 1.2 kW, a WT of 900 W, laboratory feeding the load varies throughout the day, with a bank of batteries 48 V @ 450 Ah, and the same system by adding FC 1 kW and removing the battery bank and evaluation using a set system (FC, WT, FC and battery bank), which the electrical parameters (voltage and current) are monitored, so by implementing genetic algorithms, make decisions connect and disconnect systems, the system with more elements is the best performance because the fuel cell power to supplement the battery bank, and these allow stabilize the input voltage of the inverter.

**Keywords:** Hybrid system, Fuel cell





**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Harvesting energy from leachates in microbial fuel cells using an anion exchange membrane**

**G. Hernández-Flores<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>; T. Romero-Castañón<sup>b</sup>;  
O. Solorza-Feria<sup>c</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. Código Postal 07360 Apartado Postal: 14-740, 07000 México, D.F. Tel: +52 (55) 5747 3800 ext 4321 & 4324

<sup>b</sup>Electric Research Institute. Reforma 113, Col. Palmira, C.P. 62490 Cuernavaca, Morelos, México. Tel: (777) 3623811 & 3623800

<sup>c</sup>Dept. of Chemistry, see entry<sup>a</sup>. Tel: +52 (55) 5747 3800 ext 3715 & 4473

**ABSTRACT**

The aim of this work was to evaluate the performance of single chamber microbial fuel cells (*SC-MFCs*) equipped with an anion exchange membrane, Zirfon membrane (*ZF*) with actual leachate (*lea*) as substrate, in terms of the volumetric power ( $P_V$ ) delivered and chemical oxygen removal efficiency ( $\eta_{COD}$ ). Another *MFC* equipped with a protonic exchange membrane, nafion 117 membrane (*NF*) was used as reference. The *SC-MFCs* were loaded with three different mixtures of *lea* with sulfate-reducing inocula (*SR-I*) as biocatalyst: 30% *lea* + 70% *SR-I* (period I); 70% *lea* + 30% *SR-I* (period II) and 50% *lea* + 50% *SR-I* (period III). In the **period I**, the *SC-MF* fitted with *NF* was connected to an external resistance ( $R_{ext}$ ) of 3 300  $\Omega$  and the  $P_V$  and  $\eta_{COD}$  observed were 70 mW/m<sup>3</sup> and 68%, respectively. Regarding the *SC-MF* fitted with *ZF* the obtained  $P_V$  and  $\eta_{COD}$  were 4 260 mW/m<sup>3</sup> and 63%, respectively, under an  $R_{ext}$  150  $\Omega$ . In the **period II**, the *SC-MFC* fitted with *NF* and an  $R_{ext}$  of 1 000  $\Omega$ , the  $P_V$  increased up to 100 mW/m<sup>3</sup> and the  $\eta_{COD}$  was in the order of the previous period, 64%. However, the *SC-MF* fitted with *ZF* reached a very high value of  $P_V$  (8 050 mW/m<sup>3</sup>), although the  $\eta_{COD}$  decreased to 36%. In the **period III**, again the *SC-MF* fitted with *ZF* showed encouraging values, the  $P_V$  was up to 10 380 mW/m<sup>3</sup> using an  $R_{ext}$  of 82  $\Omega$  and the  $\eta_{COD}$  was 7%, whereas the *SC-MFC* fitted with *NF* delivered a substantially lower  $P_V$  of 104 mW/m<sup>3</sup> and higher  $\eta_{COD}$  of 48%. Precipitation of salts in the cathode external surface of *MFC* equipped with *NF* could have impaired the reductive reaction of oxygen, and this, in turn, could have negatively affected its  $P_V$ . Salt precipitation apparently was not related to  $\eta_{COD}$ . In conclusion, membrane type played a significant role: the *SC-MFC* fitted with *ZF* in terms of  $P_V$  outperformed the *SC-MFC* fitted with *NF*, although the  $\eta_{COD}$  was lower, particularly in the last periods of operation. The proportion of *lea* and *SR-I* did not have a distinctive effect on *MFC* performance, whatever was the membrane type. Atypical high pH of the *lea* could partially explain the better performance of *MFCs* equipped with *ZF* over those fitted with *NF* membranes.

\* Corresponding author:

Dr. Héctor M. Poggi-Varaldo, T: 52 55 5747 3800 x 4324, Fax: 5255 5747 3313, E: r4cepe@yahoo.com



**Effect of different wavelength on the efficiency of Photosystem II and lipid synthesis in *Botryococcus braunii* UTEX 2441**

**J. Acuapan-Hernández<sup>a</sup>; H. V. Perales-Vela<sup>b</sup> ; R. O. Cañizares-Villanueva<sup>a,\*</sup>**

<sup>a</sup>CINVESTAV- IPN, Departamento de Biotecnología y Bioingeniería, Laboratorio de Biotecnología de Microalgas. Av. IPN 2508, San Pedro Zacatenco, C.P. 07360, México DF, México. Tel.: 52(55)57473800 ext. 4342. E-mail: rcanizar@cinvestav.mx

<sup>b</sup>Laboratorio de Bioquímica, Unidad de Morfología y Función, Facultad de Estudios Superiores Iztacala, Universidad Nacional Autónoma de México, Los Reyes Iztacala, Av. de los Barrios #1, Estado de México, México

**ABSTRACT**

Photosynthesis is the process by which algae, plants and cyanobacteria convert energy from light into compounds of interest such as proteins, dyes, food supplements, lipids and others; this process is regulated by the wavelength of light. Because the characteristics of the lipids produced by the chlorophycean microalga *Botryococcus braunii*, these are considered as natural sources of energy. In this study, the effect of three wavelengths ( $\lambda_{\max}$  = 460 nm,  $\lambda_{\max}$  = 518 nm,  $\lambda_{\max}$  = 634 nm corresponding to the colors of green, blue, and red respectively) on the photosynthetic efficiency and lipid synthesis in the microalga *Botryococcus braunii* UTEX 2441 was evaluated; the results were compared with respective values obtained with white light that was used as a control (white light,  $\lambda_{\max}$  = 450 and 563 nm). It was found that red light stimulated the performance of photosystem II (PSII), which was determined by changes in photosynthetic parameters: electron transport rate (ETR), quantum operating efficiency ( $\Phi$ PSII) and non-photochemical quenching (NPQ) compared to the control light. After 45 days of culture, the value of ETR,  $\Phi$ PSII, NPQ, photosynthetic efficiency and intracellular lipid content was: 16.68  $\mu\text{mol de photons m}^{-2} \text{ s}^{-1}$ , 0.66, 0.42, 9.6% y 12.5% respectively, the parameters  $\Phi$ PSII and ETR increased 8%, while the NPQ decreased 26%. The photosynthetic efficiency increased 52% and lipid content increased 38% compared to the control. These results indicate that PSII was stimulated by the red light, consequently causing a greater amount of lipid.

**Keywords:** Lipid, *Botryococcus braunii*, Wavelength, Photosystem II

\* Corresponding author:

Dr. Rosa Olivia Cañizares Villanueva, CINVESTAV- IPN, Departamento de Biotecnología y Bioingeniería, Laboratorio de Biotecnología de Microalgas. Av. IPN 2508, San Pedro Zacatenco, C.P. 07360, México DF, México. Tel.: 52(55)57473800 ext. 4342. E-mail: rcanizar@cinvestav.mx

**Trends of the production of Biohydrogen from Algae: A Review**

**D. J. Hernández-Melchor<sup>a</sup>; I. Xolalpa Alonso<sup>a</sup>; B. Camacho-Pérez<sup>a,\*</sup>**

<sup>a</sup>Área Químico-Biológicas, División de Biotecnología, Universidad Tecnológica de Tecámac, Carretera Federal México-Pachuca km 37.5, Colonia Sierra Hermosa, Tecámac.Estado de México CP. 55740, México.

\*beni.camacho@gmail.com

**ABSTRACT**

Biohydrogen is green, clean and an environmental friendly technology compared to fossil fuels. In recent years there have been studies with different microorganisms that have the capability to produce H<sub>2</sub> from organic matter (*i.e.* bacteria-*Clostridium* sp., and algae-*Chlorella* sp.) or from water oxidizing catalyzed by enzymes such as nitrogenase and hydrogenase (*i.e.* cyanobacteria- *Anabaena* sp.). For the production of H<sub>2</sub> from this phototrophic microorganisms several systems have been developed and used, known as photobioreactors (PBR). Among the latter the most important design for biomass and biohydrogen production namely the following designs: airlift, helical tubular, and flat panel. The trend to engineering development of these PBR coupled with genetically modified microorganisms improved the hydrogen production compared to conventional technologies.

The aim of this paper is to show recent advances on hydrogen production with microalgae, the subjects are the following: 1) Different microorganisms capable of producing BioH<sub>2</sub>; (biohydrogen) 2) metabolic diversity; 3) Pathways for BioH<sub>2</sub> production; 4) Enzymes responsible for production of H<sub>2</sub>; 5) Genetic engineering; 6) Reactors for BioH<sub>2</sub> production; 7) Applications of BioH<sub>2</sub>.

**Keywords:** Algae, Bioreactor, Hydrogen production, Pathway

\* Corresponding author:

B. Camacho-Pérez, 01 (55) 59 38 84 00, CP. 55740, beni.camacho@gmail.com

**Biological production of CO<sub>2</sub>-free hydrogen by anaerobic microbial mixed microflora in an upflow anaerobic sludge blanket (UASB) reactor**

**I.M.M. Moreno-Dávila<sup>a</sup>; E.B. Herrera-Ramírez<sup>a</sup>; L.J. Ríos González<sup>a\*</sup>**  
**Y. Garza-García<sup>a</sup>**

<sup>a</sup> Department of Biotechnology, Facultad de Ciencias Químicas, Universidad Autónoma de Coahuila.  
Blvd V. Carranza y José Cárdenas Valdez, Col. República Oriente. Saltillo, Coahuila, México. CP 25280  
Tel: +52 844 4155752, ext. 5. Fax: + 52 844 4159234

**ABSTRACT**

To satisfy the world's growing appetite for energy and keep our planet healthy, at least 10 TW (or terawatt) of carbon-free power has to be produced by mid-century. The process described in the present work is a CO<sub>2</sub>-free biohydrogen production in an upflow anaerobic sludge blanket (UASB). The reactor was fed with 400 ml of a mixed microbial consortium, which received acid-thermal pretreatment. The reactor was used for developed biofilms in 44 spheres covered with ixtle (natural material), and was tested at a hydraulic retention time (HRT) of 3 h using 4 L of mineral medium with glucose concentration of 20 g L<sup>-1</sup>, at initial pH 5.0 and 18°C. The hydrogen produced was sent to a gas purification device in which H<sub>2</sub> is passed through a 2M NaOH solution, this is to obtain CO<sub>2</sub>-free biohydrogen. The cumulative hydrogen production in the purification system was 52.30 mmol/h\*gSV at 230 h of fermentation. In this process was not detected carbon dioxide; and there was no methane generation due to the methanogenic pathway was inhibited, to produce hydrogen. The system had a efficiency of 81.2% in the consumption of the substrate, which for this fermentation was a synthetic medium with glucose.

**Keywords:** CO<sub>2</sub>-free biohydrogen, Anaerobic sludge blanket reactor, Biofilms

\* Corresponding author:

Leopoldo Javier Ríos González, Tel: +52 844 4155752, ext. 5. Fax: + 52 844 4159234  
Email: leopoldo.rios@uadec.edu.mx

**Review: Pretreated solid potential applied to a OFMSW biorefinery to improve the performance of hydrogen production**

**L. Romero-Cedillo<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>; T. Ponce-Noyola<sup>a</sup>; E. Ríos-Leal<sup>a</sup>;  
A.C. Ramos-Valdivia<sup>a</sup>; C.M. Cerda-García Rojas<sup>b</sup>; J. Tapia-Ramírez<sup>c</sup>**

<sup>a</sup>Departament of Biotechnology and Bioengineering, Environmental Biotechnology and Renewable Energy Group, Cinvestav-IPN, México, D.F.

<sup>b</sup>Departament of Chemistry, Cinvestav-IPN, México, D.F.

<sup>c</sup>Departament of Genetics and Molecular Biology, Cinvestav-IPN, México, D.F.

**ABSTRACT**

The organic fraction of municipal solid waste (OFMSW) has a variable composition (fluctuating contents of cellulose, hemicellulose, lignin, starch, and others). This, in turn, could lead to limited access to the biodegrading enzymes that attack, for instance, cellulose and hemicellulose. As a consequence, the yields of bioH<sub>2</sub> from dark fermentation of OFMSW could be low. Therefore it is necessary to apply a pretreatments to promote degradation/transformation of these polymers and subsequently improve bioH<sub>2</sub> production. In recent years, the pretreatment option has been extensively studied with other lignocellulosic substrates and wastes, with the main goal of removing the lignin content and to decrease the cellulose crystallinity. The most common pretreatments are mechanical, alkaline, acid diluted, thermochemical and enzymatic. Because of its high cost, the latter option is not viable to apply on a large scale. One of the challenges in the use of pretreatments is the selection of appropriate pretreatment. For example in the case of lignocellulosic residues, the most effective is the dilute acid. On the other hand, when the substrate has a lower lignin content, the alkaline pretreatment has been reported as the most adequate. There is some research where the pretreated biomass have been successfully employed to improve the performance of the processes, in specific to generate hydrogen or biomethane. In this work, we focus on describing the main pretreatments applied to OFMSW, in specific to improve the hydrogen or biomethane production.

**Keywords:** Biohydrogen, Biorefinery, Cellulose, OFMSW, Pretreatment

\* Corresponding author:

Héctor M. Poggi-Varaldo, Phone number: 5747-3800 Ext. 4321 & 4324, fax number: 5747-7002, Av. Instituto Politécnico Nacional #2508 Col. San Pedro Zacatenco, México, D.F. C.P. 07360

E-mail: r4cepe@yahoo.com

**Optimal conditions of pomace slow pyrolysis for the generation of a feedstock gas for Hydrogen production**

**M. R. Baray Guerrero; J. M. Salinas Gutierrez; M. J. Meléndez Zaragoza;  
A. López Ortiz; V. Collins-Martínez\***

Departamento de Ingeniería y Química de Materiales, Centro de Investigación en Materiales Avanzados, S.C., Miguel de Cervantes 120, Chihuahua, Chih., México, 31136, México.

**ABSTRACT**

The present research is aimed at exploring the optimal reaction conditions for the generation of a gas product, through the slow pyrolysis of pomace, to be used as a feedstock for the production of H<sub>2</sub> by the absorption enhanced reforming of methane (AER) process scheme. In order to determine conditions for rich syngas production, pyrolysis experiments were performed under in a tubular reactor, at temperature range of 150–550 °C; heating rates of 5 -20°C/min. Permanent gases (CO, CH<sub>4</sub> and CO<sub>2</sub>), aromatic tars, and chars were quantified under isothermal conditions. Results indicate that at a temperature of 400 °C and a heating rate of 5 °C/min a maximum of 71.5% W of noncondensable volatile matter (NCVM) can be obtained along with 25.4% W of condensable volatile matter (CVM), while only 3% W of residual matter (RM) was produced. At this favorable conditions (NCVM) a gas composition of 41% CO, 38% CO<sub>2</sub> and 21% CH<sub>4</sub> was generated. A thermodynamic analysis of this product gas was performed under the steam reforming of methane combined with CO<sub>2</sub> solid absorption (AER) by CaO for the production of high purity H<sub>2</sub>. Thermodynamic calculations using a steam to methane ratio (S/C) of 4 and 1 mol of CaO/mol of CH<sub>4</sub> indicate that a maximum H<sub>2</sub> production is achieved at 690 °C along with a composition of 74.1 % H<sub>2</sub>, 16.2% CO, 7.6% CO<sub>2</sub> and 2.1% CH<sub>4</sub> with no carbon formation.

**Keywords:** Pomace pyrolysis, Hydrogen production, CO<sub>2</sub> capture

\* Corresponding author:

Virginia Collins Martinez, phone: +526144391129; e-mail: virginia.collins@cimav.edu.mx



**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Synthesis and characterization of membranes based on agar-agar-KCl**

**G. Hernández-Flores<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>; V. Compañ<sup>b</sup>;  
O. Solorza-Feria<sup>c</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Apartado Postal: 14-740, 07000 México, D.F. Tel: +52 (55) 5747 3800 ext 4321 & 4324

<sup>b</sup>Dpto. Termodinámica Aplicada, ETSII, Universidad Politécnica de Valencia, 46022 Valencia, Spain

<sup>c</sup>Dept. of Chemistry, ibídem. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. Código Postal 07360; Tel: +52 (55) 5747 3800 ext 3715 & 4473

**ABSTRACT**

In general, the use of separators or membranes in microbial fuel cells (*MFCs*) improve the *MFC* performance. Nafion, hydrated perfluorosulfonic acid membranes, are the separators typically used in *MFCs* and fuel cells because of their good characteristics. However, their relatively high cost has been identified as a deterrent for *MFC* fabrication and scale up. Thus, the goal of this work was to develop and characterize new types of low cost agar membranes (*LCAM*). Three sets of membranes were prepared. The first one used agar in variable concentrations 2 to 8% (w/v). Both the proton conductivity (*PC*) and O<sub>2</sub> permeability (*OP*) increased with the agar concentration up to 4% agar, beyond this point the *PC* levelled-off ( $2.43 \times 10^{-3}$  S/cm) whereas the *OP* continued to increase. A second set of membranes was made with agar spiked with KCl, testing different concentrations of agar. At a fixed concentration of 10% KCl and increasing the agar concentration from 2% to 8%, both the *PC* and *OP* increased with the increase of the agar concentration, however the presence of the KCl slightly negatively affected the latter. A third set of membranes was made with a fixed concentration of 2% agar and increasing the KCl concentration from 2% to 10%. It was observed that *PC* did not significantly increase with salt concentration whereas the worst values of *OP* were observed. This suggests that agar presence and concentration would play a significant role on the increase of proton conductivity, instead of the expected influence of the salt. In general the electrical resistance *R* exhibited by all *LCAM* was encouragingly low. The lowest *R* observed in the first set was 6  $\Omega$  for the membrane with agar 2%; the *R* increased with the agar concentration. In the 2<sup>nd</sup> set of *LCAM*, the membrane with agar 6% + KCl 10% showed the lowest resistance (4  $\Omega$ ) and the best proton conductivity  $7.10 \times 10^{-3}$  S/cm. However, in the third set of *LCAM*, there was no evidence of consistent trends of the properties; we found that the proton conductivities were the lowest of all the sets. Selected *LCAMs* have been tested in *MFCs* for the treatment of actual leachate and municipal wastewater, with encouraging results and typically better than those of cells fitted with Nafion separators.

**Keywords:** Agar membranes, Agar-KCl membranes, Microbial fuel cell, Nafion, Proton conductivity, Oxygen permeability

\* Corresponding author: Prof. Dr. Héctor M. Poggi-Varaldo 52 55 5747 3800 x 4324, r4cepe@yahoo.com





**Synthesis of biodiesel and value-added products from glycerol using sodium and lithium silicate**

**A. Sacristán<sup>1</sup>; I. C. Romero-Ibarra<sup>2\*</sup>; H. Pfeiffer<sup>1</sup>**

<sup>1</sup> Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México. Ciudad Universitaria s/n Coyoacán 04510, México D. F.

<sup>2</sup> Universidad Autónoma Metropolitana - Iztapalapa, San Rafael Atlixco No. 186, Col. Vicentina, 09340, A.P. 55-534, México, D. F. e-mail: icromeroib@conacyt.mx

**ABSTRACT**

The alarming trends in energy demand and the finite nature of fossil fuel reserves have motivated the search for energy sources more sustainable. In this regard, biodiesel can provide a significant contribution in the energy independence. The production of biodiesel generates millions of tons of crude glycerol waste per year (generally, 10 to 20% of the total volume of biodiesel produced is made up of glycerol) and this amount is growing rapidly along with the dramatic growth of biodiesel industry. Thus, new markets or new applications of glycerol such as converting it into value-added products would have to be explored.

In this work, sodium and lithium silicates ( $\text{Na}_2\text{SiO}_3$  and  $\text{Li}_2\text{SiO}_3$ ) were synthesized via a solid-state reaction and evaluated as potential catalytic materials. The structure and microstructure of the catalysts were characterized using X-ray diffraction, scanning electron microscopy and  $\text{N}_2$  adsorption. Then, both silicates were tested as a basic catalyst for the production of biodiesel from transesterification reaction. The influence of some parameters was investigated, such as the reactant concentrations (molar ratios), reaction time, temperature and re-use of the catalyst. The maximum FAME conversion efficiency was ~99% at 1 h of reaction time and 3wt% of catalyst. The cyclic behavior revealed that the catalyst had a relatively stability. Besides, the same silicates were performed as catalysts on synthesis of the by-glycerol transformation into different valued-added products. The products were characterized using infrared spectroscopy, gas chromatography coupled to mass spectrometry and proton nuclear magnetic resonance. The use of  $\text{Na}_2\text{SiO}_3$  is a good option to test as catalyst transesterification reaction in the reutilization with high yields. A combination of biodiesel production with subsequent glycerol conversion to value-added products, as synthesis gas ( $\text{CO} + \text{H}_2$ ), by directly using the heterogeneous catalyst is a good option to reduce cost and pollution.

\* Corresponding author:

I. C. Romero-Ibarra, UAM- Iztapalapa, San Rafael Atlixco No. 186, Col. Vicentina, 09340, A.P. 55-534, México, D. F. E-mail: icromeroib@conacyt.mx

**Hybrid membranes for microbial fuel cells**

**G. Hernández-Flores<sup>a</sup>; V. Compañ<sup>b</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>;  
O. Solorza-Feria<sup>c</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Apartado Postal 14-740, 07000 México, D.F., Mexico Tel: +52 (55) 5747 3800 ext 4321 & 4324

<sup>b</sup>Dpto. Termodinámica Aplicada, ETSII, Universidad Politécnica de Valencia, 46022 Valencia, Spain

<sup>c</sup>Dept. of Chemistry Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Apartado Postal 14-740, 07000 México, D.F., Mexico Tel: +52 (55) 5747 3800 ext 3715 & 4473

**ABSTRACT**

Protonic exchange membranes (*PEM*) such as Nafion 117, are the membranes commonly used as membranes in microbial fuel cells (*MFCs*) and fuel cells. However, costs are very high. The aim of this work was to prepare and characterize a set of hybrid membranes (*HM*) made of mixtures of synthetic polymers and agar in the context of their possible application in *MFCs*. Tested membranes were: agar 2% - 1% Nafion (*M1*); agar 2% - 2% Nafion (*M2*); one film of (Poly vinyl alcohol) *PVA* + agar 2% (*M3*); double film of *PVA* + agar 2% (*M4*); sulfonated poly ether ether ketone (*SPEEK*)/*PVA* 12 steps 5% *SPEEK*/*DMAC* (inmersed in agar 2%) (*M5*); Nafion/*PVA* (inmersed in agar 2%) (*M6*) and Ammealing 140 °C 1h 100 kg/cm<sup>2</sup> (inmersed in agar 2%) (*M7*).

The proton conductivity *PC* observed in our membranes were (S/cm): *M1*, 1.54×10<sup>-3</sup>; *M2*, 2.12×10<sup>-3</sup>; *M3*, 4.00×10<sup>-4</sup>; *M4*, 4.60×10<sup>-4</sup>; *M5*, 1.08×10<sup>-3</sup>; *M6*, 1.38×10<sup>-3</sup> and *M7*, 9.83×10<sup>-4</sup>.

On the other hand, regarding the oxygen permeability *OP* (barrer), the lowest values were observed for *M1* and *M2* whereas *M7* exhibited the highest value 2.01×10<sup>-10</sup> [cm<sup>3</sup> (STP oxygen) cm<sup>2</sup>/cm<sup>3</sup> (material) s mm Hg×10<sup>-11</sup>]. *M1* and *M2* also displayed the highest *PC*. The presence of *PVA* in the material of the membranes seemed to lower both the *OP* and *PC*. On the other hand, those membranes with Nafion in their composition showed a higher *PC*, that varied nearly in direct proportion to Nafion content. In general, the *HM* analyzed in this work showed encouraging values and are options to use in *MFCs* or fuel cells, although no membrane type tested in our work exhibited simultaneously the desirable profile, that is, the highest *PC* and the lowest *OP*.

**Keywords:** Hybrid membranes, Microbial fuel cell, Nafion 117, Proton exchange membrane

\* Corresponding author: Professor Dr. Héctor M. Poggi-Varaldo T: 52 55 5747 3800 x 4324; E : r4cepe@yahoo.com

**Effect of the phenolic compounds in the sugar cane bagasse  
saccharification for the lignocellulosic ethanol production**

**E. González-Bautista<sup>a</sup>; J. C. Santana-Morales<sup>a</sup>; A. C. Ramos-Valdivia;  
H. M. Poggi-Varaldo<sup>a</sup>; T. Ponce-Noyola<sup>a,\*</sup>**

<sup>a</sup>Departamento de Biotecnología y Bioingeniería. Centro de Investigación y de Estudios Avanzados del  
Instituto Politécnico Nacional, México, D.F., C.P. 07360.

**ABSTRACT**

One of the most important steps for the production of second-generation ethanol from agro-industrial waste is the saccharification process. However during enzymatic hydrolysis, secondary metabolites of phenolic nature are released which are part of the lignin structure in the plant cell walls. This phenolic compounds work such as auxins compounds which are capable of inhibiting the growth of microorganisms when inhibit enzymes such as holocellulases. In this way a pretreatment should remove these inhibitory compounds. However even after pretreatment phenolic compounds still remain that may negatively affect the enzymatic activity. There are certain soluble polymers that can prevent such inhibition by their physicochemical properties and their ability to chemical-adsorb phenolic compounds in their structure. In this work we studied the capacity of polyethyleneglycol (PEG) and polyvinylpyrrolidone (PVP) to prevent enzyme inhibition of xylanases and CMCase of *Cellulomonas flavigena* strain PR-22 during saccharification of sugar cane bagasse pretreated with sodium hydroxide (NaOH). We evaluated the inhibition effect of phenolic compounds on the enzymatic activity of xylanases and CMCase. For this purpose a concentrated extract whit phenolic compounds was prepared from the hydrolysis of raw sugarcane bagasse. This extract was added to the reaction mixture at different concentrations and then we analyze the remaining activities of xylanases and CMCase after incubating at optimal conditions for each enzyme activity. We found 77% inhibition of xylanase activity with 100 µg of phenolic compounds and 66% in CMCase activity with 50 µg of phenolic compounds. PEG and PVP were added at 0.4% (p/v) to *C. flavigena* PR-22 cultures growing in sugarcane bagasse in order to avoid the effect of inhibition of the phenolic compounds. The addition of PEG avoid CMCase inhibition by phenolic compounds obtaining 92% of the original activity after the saccharification, while in the negative control this activity only reached 44%. On the other hand the PVP favor the xylanase activity in 62% and in the negative control only got 30% of the original activity. Cultures where PVP was added, accumulated 34% more reducing sugars than in control cultures, while cultures with PEG produced 30% more than its negative control.

**Keywords:** Ethanol production, Phenolic compounds, Saccharification, Holocellulases

\* Corresponding author:

Dra. Teresa Ponce Noyola +52 (55) 5747 3800 ext. 4317 E: tponce@cinvestav.mx

## **Separators in microbial fuel cells: A Review**

**G. Hernández-Flores<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. Código Postal 07360 Apartado Postal: 14-740, 07000 México, D.F. Tel: +52 (55) 5747 3800 ext 4321 & 4324

### **ABSTRACT**

Microbial fuel cells (*MFCs*) are electrochemical devices focused in electricity generation and organic matter removal from wastewater under anoxic environments. The *MFCs* configuration is similar to fuel cells, both have an anode, cathode, and needs a fuel and proton exchange membrane. However, in *MFCs* the fuel generally are wastewater or leachates, i.e., wastes, whereas in fuel cells, hydrogen is the fuel. Membranes in *MFCs* could represent around the 40% of the *MFC* total cost. It is one of the challenges to scaling up *MFCs*, find alternative membranes or separators with low cost and good electrochemical characteristics. The goal of this work is to critically review the state of the art on membranes in *MFCs*. The scope of this review includes (i) the different membranes used in *MFCs*, (ii) costs and performance of typical membranes used, (iii) configuration of membranes in *MFCs*, (iv) membraneless *MFCs*, and (v) perspectives on *PEMs*.

Thus, there are at least 20 different membranes or separators used in *MFCs*, from the primitive salt bridges to synthetic polymer-based membranes, passing by ceramic and special materials separators. A survey of the costs of membranes/separators indicate the following ranges, depending on the type (in USD/m<sup>2</sup>): anion exchange membranes AMI 7001, 80-83; cation exchange membranes such as CMI-7000 200, and Nafion 117, 1400-2200; plastic (polypropylene) mesh, 13-26; stainless steel mesh, 80-135; ultrafiltration membranes, 350, and J-cloth, 400.

Unfortunately, studies focused on low cost and or natural polymers for *PEM* are still scarce. Alternatively, in some works, the *MFCs* have been operated without a membrane. Yet it was found that the coulombic efficiency substantially decreased. Because of the type of membrane affects the performance and the total cost of the *MFCs*, it is recommended to increase research efforts to develop new, more economic membranes that exhibit good properties and allow for good cell performance at the same time. The knowledge gathered in the review of membranes for *MFCs* undoubtedly will give useful insights on future research needs in this area. Our overview will also discuss these issues.

**Keywords:** Coulombic efficiency, Microbial fuel cell, Protonic exchange membrane, Separators

\*Corresponding author:

Professor Dr. Héctor M. Poggi-Varaldo; T: 52 55 5747 3800 x 4324 ; E: r4cepe@yahoo.com



**Biocathodes, a bioelectrochemical technology for electricity generation  
and effluents treatment: a review**

**J. E. Borbolla-Gaxiola<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F. Código Postal 07360 Apartado Postal: 14-740, 07000 México, D.F. Tel: +52 (55) 5747 3800 ext 4321 & 4324.

**ABSTRACT**

Among the different alternative energy technologies, the microbial fuel cells (*MFC*) have drawn considerable attention, due to its capacity to produce electrical energy from wastes and biomass. Many efforts have been verted into the research on the subject, nevertheless, the majority of the studies have been focused on the development of *MFC* with abiotic cathode. The implementation of biochatode in a double-chamber *MFC* system exhibits several advantages over the traditional abiotic cathode systems, including the reduction of contruction and operation costs by eliminating the use of expensive abiotic catalysts, such as platinum, and the addition of external electron transfer mediators; additionally. It also offers the opportunity to use the reductive metabolim of the biocathode to biologically reduce different electron acceptors that could be pollutants of conern, such as nitrate and others. This reductive capacity has been used in the treatment of effluents with oxidized contaminants, like chlorinated xenobiotics. Increasing the range of reducible contaminants is a crucial factor to improve the sustainability and feasibility of the biocathode based *MFC*.

Previous work has focused on the biocathode materials, the electron transfer mechanisms involved and the advances in denitrification and azo dyes degradation. This review encompasses the state-of-the art of the biocathode technology in the treatment of contaminated effluents, the diversity of contaminants studied to date, energy production, enrichment of inocula used as biocatalysts, and other conditions used in the process. The knowledge of the whole range of contaminants treated as well as other topics can provide insightful perspectives on the future direction of reaserch in this area, and improve the effectiveness and usefulness of the technology. These issues will also be discussed in this review.

**Keywords:** Biocathode, Bioelectrochemistry, Energy, Microbial fuel cell

\* Corresponding author:

Professor Dr. Héctor M. Poggi-Varaldo; T: 52 55 5747 3800 x 4324; E: r4cepe@yahoo.com





**A review on microbial fuel cell technology for  
soil and sediment remediation**

**K. B. Sánchez-López<sup>a</sup>; H. M. Poggi-Varaldo<sup>a, b,\*</sup>**

<sup>a</sup>Nanoscience and nanotechnology program, Cinvestav-IPN, México, D.F.

<sup>b</sup>Departament of Biotechnology and Bioengineering, Environmental Biotechnology and Renewable Energy Group, Cinvestav-IPN, P.O.Box 14-740, Cd. de México D.F. 07000, México

**ABSTRACT**

The need for remediation of soils and sediments contaminated with pollutants of concern has led to the development of new technologies such as those represented by the interface between biotechnology and electrochemistry, i.e., microbial fuel cells (*MFCs*). The objective of this work is to critically review the development and contribution of *MFC* technology to the environmental remediation of solid matrices. This review encompasses the following subjects: (i) pollutants; (ii) co-substrates used; (iii) cell configurations; (iv) types of soils; and (v) miscellaneous issues.

A great variety of pollutants from petroleum hydrocarbons to chlorinated organic compounds and pesticides have been successfully treated in *MFCs*. On the other hand, research on remediation of soils polluted with emerging pollutants that affect human health using *MFC* is still scarce. It has been reported the use of co-substrates may affect or benefit the process, the co-substrate most used is glucose for difficult compounds to oxidize as azo dyes, followed by ethanol, pyruvate, acetate, among others. On the other hand, hydrocarbon remediation does not usually need co-substrate. *MFC* configurations so far show that there two main types of arrangements: *in situ* cells (anodes buried in the solid matrix) and the more conventional *ad situ* cells (two and one chamber ones). In spite of possible lower costs of the first type, the second ones offer a better process control and higher treatment rates. Regarding the *ad situ* type it was shown that placing the anode horizontally can optimize the process. The *ad situ MFC* approach can treat a wide range of soils, from sandy to very “heavy” soils (high contents of both clay and organic matter). Therefore, *MFC* remediation could be more advantageous than the very popular *in situ* remediation that is limited by low hydraulic conductivity and low permeability of soils. Interestingly, addition of  $\text{Fe}(\text{OH})_3$  stimulated humification of organic matter in sediments treated in *MFCs*. Also selected physico-chemical properties of sediment organic matter such as the humification-like process was stimulated when electrical current was produced.

Yet, several research areas still need to be started or reinforced, such as the studies on technology combination nanotreatment plus *MFC*; soil remediation assessment in *MFC* equipped with biocathodes for specific pollutants that could be removed by reduction; and evaluation of sustainability of the technology by application of Life Cycle Analysis and system analysis, *inter alia*.

**Keywords:** Microbial fuel cells, Soil, Sediment, Remediation

\* Corresponding author:

Héctor M. Poggi-Varaldo, T: 5255 5747-3800 Ext. 4321 & 4324, E: r4cepe@yahoo.com



**Alternative membranes to replace Nafion membranes  
in microbial fuel cells**

**G. Hernández-Flores<sup>a</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>; O. Solorza-Feria<sup>b</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F., C. P. 07360 Apartado Postal: 14-740, 07000 México, D.F.

<sup>b</sup>Dept. of Chemistry, *ibidem*. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F., C. P. 07360 Apartado Postal: 14-740, 07000 México, D.F.

**ABSTRACT**

The aim of this work was to compare the performance of microbial fuel cell (*MFC*) fitted with alternative, low cost membranes (*AMs*). Lab scale single chamber *MFCs* were loaded with sulfate-reducing inocula as biocatalyst and leachate from dark fermentation of organic wastes as substrate. The *MFCs* were fitted with either an agar membranes *M2* (2% agar), *M6* (6% agar), a hybrid membrane made of agar and Nafion *MH*, or the control Nafion 117 membrane (*NF-117*).

We found that the internal resistances ( $R_{int}$ ) were generally low for all the cells. The lowest  $R_{int}$  corresponded to alternative membranes *M6* and *MH* with a value *ca.* 90  $\Omega$ . So, results of  $R_{int}$  tend to favour the *AMs*. The costs of these membranes were only 2.5 to 6% of the cost of the *NF-117* one. However, the powers delivered by *MFC* fitted with *AMs* were 4 to 40% (weighed average 28%) of the power of the cell fitted with the conventional *NF-117*. In spite of the reduced power, the *AMs* still exhibited a higher Power/Cost ratio (0.9 to 4.4. mW/US\$) than that of the *NF* membrane (0.23 mW/US\$.)

We should highlight that the *AMs* do not require the conditioning treatment with hazardous chemicals typical of *NF-117*. Therefore, there is another competitive edge of *AMs* in the form of avoided costs of chemicals and hazardous waste disposal.

**Keywords:** Leachate, Proton exchange membrane, Low cost membrane, Power/cost ratio, Microbial fuel cell, Internal resistance

\* Corresponding author:

Professor Dr. Héctor M. Poggi-Varaldo; T: 52 55 5747 3800 x 4324 ; E: r4cepe@yahoo.com



**Microbial fuel cells fed with municipal wastewater and leachates**

**G. Hernández-Flores<sup>a,\*</sup>; H. M. Poggi-Varaldo<sup>a,\*</sup>**

<sup>a</sup>Environmental Biotechnology and Renewable Energies R&D Group, Dept. of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional. Av. Instituto Politécnico Nacional 2508, Col. San Pedro Zacatenco, Delegación Gustavo A. Madero, México D.F., C. P. 07360 Apartado Postal: 14-740, 07000 México, D.F.

**ABSTRACT**

The goal of this work was to evaluate the extent of treatment and bioelectricity generation in microbial fuel cells (*MFC*) fed with municipal wastewater (*MWW*) and leachate from the Mexico City landfill “Bordo Poniente” section 1 and 4 (*L-1* and *L-4*). Leachates exhibited a medium organic strength and interestingly, their pH was alkaline.

An air-cathode, single chamber *MFC* was loaded first with *MWW* and sulfate-reducing consortium as inoculum (*SR-In*). During the batch operation with *MWW* an external resistance of 330  $\Omega$  was used and an average removal of organic matter of 60% ( $\eta_{COD}$ ) and 4% coulombic efficiency (*CE*) were achieved, along with average volumetric power ( $P_v$ ) of 273  $\text{mW m}^{-3}$ . Afterwards, two repeated more batches were carried out; where the *CE* significantly increased up to 48% whereas a  $\eta_{COD}$  slightly improved of 78% was reached in the last two periods. A 2<sup>nd</sup> experiment was carried out using a mixture of *MWW* and *L-4* aged leachate from the Mexico City landfill plus *SR-In*. Two more operation periods were carried out loading *L-4* y *L-1* as substrate into the *MFC*. When a mixture of *L-4* and *MWW* was loaded into the cell, the highest value of  $\eta_{COD}$  was observed in this work, i.e., 86%. Afterwards, using 100% *L-4*, the  $\eta_{COD}$  and the *CE* achieved were 53% and 15%, respectively, whereas a  $P_v$  of 490  $\text{mW m}^{-3}$  was observed. It seems that treatment of combined leachate and *MWW* had a beneficial effect on *MFC* performance. To the best of our knowledge this is the first report on the use of *MFCs* to the treatment of atypical leachates from Mexico City’s landfill and its mixtures with *MWW*.

**Keywords:** Remediation, Municipal wastewater, Leachates, Microbial fuel cells, Coulombic efficiency, Organic matter removal

\* Corresponding author:

Professor Dr. Héctor M. Poggi-Varaldo; T: 52 55 5747 3800 x 4324 ; E: r4cepe@yahoo.com

**Used disposable diapers as substrate for hydrogen production:  
Effect of temperature and diaper conditioning**

**P. X. Sotelo-Navarro<sup>a</sup>; H. M. Poggi-Varaldo<sup>b,\*</sup>; S. J. Turpin-Marion<sup>a</sup>;  
R. M. Espinosa-Valdemar<sup>a</sup>; A. Vázquez-Morillas<sup>a</sup>; M. Beltrán-Villavicencio<sup>a</sup>**

<sup>a</sup> Department of Energy, Sustainable Technologies Laboratory, UAM-A, México, D. F.

<sup>ba</sup> Department of Biotechnology and Bioengineering, Environmental Biotechnology and Renewable Energy Group, Cinvestav-IPN, México, D.F.

**ABSTRACT**

The aim of this work was to evaluate the effect of temperature (35 and 55 °C) as well as diaper conditioning on bioH<sub>2</sub> production in batch fermentation of *used* disposable diapers. The cumulative bioH<sub>2</sub> production was evaluated in batch mini-reactors for whole diapers (WD), diapers without plastic components (PSD), and manually separated diaper (MSD) that eliminated both plastic and feces, and reactors containing only inoculum as a control. All diaper samples were ground in a hammer mill. The mini-reactors had a 50 mL capacity. Substrate was set at 25% of total solids and inoculum was loaded at a ratio of 10% dry weight basis. When the bioH<sub>2</sub> production reached a plateau, the headspaces of the reactors were flushed with N<sub>2</sub> and the reactors were re-incubated without feeding substrate nor inoculum, following a procedure known as AF-IV (anaerobic fermentation with intermittent venting).

Results showed that bioH<sub>2</sub> cumulative production was higher at 55 °C than at 35 °C, which may be due to the limited growth of hydrogen consumers and faster metabolic activity of the bacteria reported for the thermophilic range. Interestingly, on the average the cumulative bioH<sub>2</sub> production followed the order WD > MSD > PSD. We expected higher cumulative bioH<sub>2</sub> productions for the diapers without the plastic components because the latter are not biodegradable and could account for ca. 30% of the diaper weight. Although we presented the main effect of both factors in our experiment there was a significant interaction temperature-diaper conditioning.

In general, our tests have shown low yields in the production of H<sub>2</sub> at both temperatures compared to those obtained in the literature for organic waste. There is preliminary evidence that sodium polyacrylate (SAP; a polymer that is used as urine super absorbent in disposable diapers) could have inhibited to some extent the biohydrogen production. Research is ongoing to overcome this effect and increase the suitability of used disposable diapers as substrate for bioH<sub>2</sub> generation.

**Keywords:** Hydrogen production, Disposable diaper, Fermentation

\* Corresponding author:

Héctor M. Poggi-Varaldo, Phone number: 5747-3800 Ext. 4321 & 4324, fax number: 5747-7002, Av. Instituto Politécnico Nacional #2508 Col. San Pedro Zacatenco, México, D.F. C.P. 07360. E: r4cepe@yahoo.com



## **Control and power conditioning**

**Energy management system for a hybrid hydrogen-solar  
sustainable house**

**O. Aguado-Sánchez<sup>a,\*</sup>; R. de G. González-Huerta<sup>b,\*</sup>; D.J.Cortés-Rodríguez<sup>a</sup>**

<sup>a</sup>Instituto Politécnico Nacional, ESIME Culhuacan, Av. Santa Ana No. 1000, 14430, Mexico City, Mexico

<sup>b</sup>Instituto Politécnico Nacional, ESQUIE, Unidad Profesional Adolfo López Mateos Edificio No. 7, 07738 Mexico City, Mexico.

**ABSTRACT**

The advantage of using hybrid systems compared with independent sources such as wind turbines or photovoltaic grid is the possibility of make synergy, making a robust system that can ensure the power supply when the user demands it and the ability to store excess energy in different weather conditions.

In this paper a system for an energy management of a hydrogen-solar hybrid sustainable house is described. The house has three different power sources that consist of two proton exchange membrane fuel cells, a rigid photovoltaic panel grid and a flexible photovoltaic panel grid. All these power sources have different characteristics that result in different power capabilities therefore a control system is necessary to interconnect these sources to ensure proper distribution of energy as well as take care the function of each device on the system. To this end, strategic electric signals are measured and connected to a programmable logic controller, taking into account the system state, and energy requirements. The developed algorithm performs switching actions of relays to separate or join the different voltage buses depending on the loads demand, in order to feed an specific bus with more power. The algorithm includes a manual mode that allows the user to select different available buses with the aim of avoid energy blackouts in priority loads distributed in the home. Although the energy management system developed in this paper has been designed for three sources, it can be extended to more different power sources and more output buses.

**Keywords:** Power management, Programmable logic controller, Hydrogen fuel cells, Solar cells

\* Corresponding author:

Octavio Aguado Sánchez, Tel. +52-55.4524.4916, octavio.oas@gmail.com

## **Control implementation of a DC-DC energy router for renewable sources**

**D. Navarro Durán<sup>a,\*</sup>; E. Perez Hernandez<sup>a</sup>; J. Resa Trejo<sup>a</sup>; D. Cortes Rodriguez<sup>a</sup>**

<sup>a</sup>Instituto Politecnico Nacional Superior School of Electrical and Mechanical Engineering Av. Santa Ana No. 1000 Mexico City 04430, Mexico Teléfono 01 55 5624 2000. david.navarro.d@gmail.com

### **ABSTRACT**

It is undeniable that renewable energies are the sources of the future. The energy demand will continue to grow and if it is supplied by fossil fuels a negative impact will cause complications as pollution and climatic change. On the other hand, the renewable energies has the disadvantage of being dependent on the environmental conditions. As a consequence a single renewable energy cannot supply the energy demanded all the time, hence a combination of the renewable sources is the best approach to this end. Many approaches have been developed to combine different power sources, but in some circumstances the energy requirements is not fully harnessed.

A better approach to improve the energy management is to develop a power electronic converter which allows sources from different characteristics to cooperate simultaneously to power a load. The device that achieves this goal has been called “energy router” by some researchers. Multi-input power electronic converters have been studied because with the proper control they can accomplish the energy router goal. There are many power electronic converters which can perform energy routing, but many of those topologies complicate the controller design.

In this paper a multi-input buck converter is implemented as an energy router. To achieve the energy transfer a sliding mode control is developed, considering  $\alpha$  parameters to determine the energy provided by each source. To evaluate the controller performance a simulation is presented, and favorable results were obtained under load variations and different energy rating conditions. To go further a 50 W prototype was designed to implement the controller, the experimental results show a stable control with good voltage output regulation.

**Keywords:** Renewable sources, Power energy Router, Nonlinear control, Energy transfer

\* Corresponding author:

D. Navarro Durán, Instituto Politecnico Nacional Superior School of Electrical and Mechanical Engineering Av. Sta. Ana No. 1000 Mexico City 04430, Mexico Teléfono 01 55 5624 2000, david.navarro.d@gmail.com

## **Cascaded multilevel inverter for fuel cell applications**

**V. M. Sanchez<sup>a,\*</sup>; J. C. Rosas Caro<sup>b</sup>; A. Valderrabano-Gonzalez<sup>b</sup>**

<sup>a</sup>Universidad de Quintana Roo, Boulevard Bahía s/n, Chetumal, Q. Roo, México, CP 77019

<sup>b</sup>Universidad Panamericana UP campus Guadalajara, Circunvalación Poniente #49, Zapopan, Jalisco, México, CP 45010.

### **ABSTRACT**

Fuel cell generation systems are expected to see a significant increase in their practical usage due to several advantages they offer over conventional generation systems. However, fuel cells generate DC power so that a power conversion is required in order to be interconnected with AC power systems. Multilevel converters allow obtain a desired AC voltage by adding several DC voltages. This work presents a single-phase multilevel boost cascaded inverter which employs only one DC power source. The converter is ideal for Fuel Cell applications as inverter stage in energy generation or grid integration. Multilevel inverter proposed uses a floating capacitor in order to generate a DC voltage level which is added to the main DC source. Besides, proposed switching procedure for the multilevel inverter keeps the capacitor voltage equal to the DC source without a complex control task. Operating principle, analysis and simulation results of a 5-level cascaded multilevel inverter are shown.

**Keywords:** Multilevel inverter, Fuel cells, Power conditioning converters, Renewable systems

\* Corresponding author:

Víctor M. Sánchez Huerta. Tel: +52 9838350300, Fax: +529838329656. Email: vsanchez@uqroo.edu.mx

**Design and implementation of electronic control system to enriched gasoline with oxi-hydrogen in internal combustion engines**

**B. A. Grunstein-Ramirez<sup>a,\*</sup>; E. Ruiz-Hernandez<sup>a</sup>; G. D. Meneses-Rayas<sup>a</sup>;  
R. de G. González Huerta<sup>b</sup>**

<sup>a</sup>UPIITA-IPN, Av. Instituto Politecnico Nacional 2580, C.P. 07340, México D.F.

<sup>b</sup>IPN-ESIQIE, Lab. Electroquímica y Corrosión, C.P. 07738, México D.F.

**ABSTRACT**

Internal combustion engine vehicles are an important pollution source. Because of this, several research groups are implementing systems that reduce the use of hydrocarbon, in the first stage the gasoline enrichment with alternative fuels such as ethanol, hydrogen, and others have been considered. In this paper, it has been developed an electronic control system which regulates oxy-hydrogen gas production generated in-situ,  $\text{NOH}_2$  (mixture of hydrogen and oxygen at 2:1 rate, at normal conditions, 1 atm and 0 °C) in order to enrich the fuel and reduce the gasoline amount consumed by the engine and reduce the pollution gas emission. The gas generation was produced by two alkaline reactors in parallel-series arrangement, which had energy consumption from 60 to 500 W with 50 to 65% of efficiency. Hydrogen storage system was not required because of the in-situ generation. Main goal of the electronic control system is regulate oxy-hydrogen volume fractions in the total intake air flow at 5% which is fed to combustion chamber (125 cc engine) from 1000 to 2500 rpm. Oxi-hydrogen mass flow was determined by motor thermodynamic calculations (Otto cycle). The electronic control system allowed gas ( $\text{NOH}_2$ ) production from 0.6 to 2.5 L/min. Using Faraday laws, the  $\text{OH}_2$  gas mass flow was indirectly controlled by current regulation applied to reactors, ranging from 10 to 40 A. This developed system allowed to save 9.7% of gasoline volume and the oxy-hydrogen enrichment contributed to decrease  $\text{CO}_2$  and CO emissions, being lower than the standard gasoline engine.

**Keywords:** Hydrogen, Combustion engines, Power electronic, Alkaline electrolysis, Electronic control

\* Corresponding author:

Bernardo A Grunstein Ramírez, 52 (777) 523 8400, b\_grunstein@hotmail.com.com



## **Policies, economy and market strategies**



## **Infraestructure analysis of the hydrogen refueling station in Mexico**

**N. Nuñez García; D. Morales Herrera; A. Zaragoza González; M. Sanchez Vazquez;  
R. de G. González Huerta \***

IPN-ESIQIE, Laboratorio de Electroquímica y Corrosión, UPALM, CP 7738, DF, México

### **ABSTRACT**

Finding a new source of energy that is renewable and generates a technological impact is needed; one that will benefit the country in terms of growth and development of new technology and social structures. Hydrogen, as an alternative source of energy, is proposed to be used as an energy vector. Studies and articles worldwide claim that the use of hydrogen is not a luxury but an absolute need. The implementation of hydrogen is linked to the development of infrastructure for the production, storage and recharging, plus technical specifications that must be considered. Mexico is seen as a country 90% dependent on fossil fuels, it is currently in an initial phase for the implementation of alternative energy, to reduce the bad environmental impact.

To gain acceptance of the use of hydrogen, a study about comprising implementing of hydrogen stations is being conducted. The research is based on studies reported in the US, Germany, Spain, Japan and Brazil which show a line of investigation that began 10 years ago for the use of hydrogen as fuel in transport systems. The tested technology involves the development of three types of hydrogen refueling stations: 1) On-Site, 2) Pipeline delivery 3) Liquid or gaseous hydrogen delivery. The proposal presented in this research is based on the implementation of an On-Site station in Mexico, where technical, economic and geographic characteristics are necessary for the installation of a safe hydrogen refueling in cars and buses. With this investigation we pretend to impulse our country to a new route of clean technology.

**Keywords:** Refueling station, Infrastructure, Hydrogen, Safety, Implementation

\* Corresponding author:

Rosa de Guadalupe González Huerta, (+52) 55 57296000 x 54246, rosgonzalez\_h@yahoo.com.mx

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Public policy performance for social development: solar energy approach  
to assess technological outcome in Mexico City Metropolitan Area**

**A. R. Arenas-Aquino<sup>a,\*</sup>; Y. Matsumoto-Kuwabara<sup>b</sup>; M. Kleiche-Dray<sup>c</sup>;  
R. Baquero-Parra<sup>d</sup>; C. González-Brambila<sup>e</sup>; G. Isunza-Vizuet<sup>f</sup>;  
H. M. Poggi-Varaldo<sup>g</sup>**

<sup>a</sup>Department of Science Methodology, Centro de Investigación y de Estudios Avanzados, 2508 Instituto Politécnico Nacional, San Pedro Zacatenco, Distrito Federal, 07360, Mexico.

<sup>b</sup>Department of Electrical Engineering, *ibid.*

<sup>d</sup>Department of Physics, *ibid.*

<sup>g</sup>Department of Biotechnology baDepartament of Biotechnology and Bioengineering, Environmental Biotechnology and Renewable Energy Group, Cinvestav-IPN, México, D.F.

<sup>c</sup>IRD - Ceped & IFRIS, 19 Rue Jacob, Paris, 75006, France.

<sup>e</sup>Academic Department of Administration, Instituto Tecnológico Autónomo de México, 1 Río Hondo, Progreso Tizapán, Distrito Federal, 01080, Mexico.

<sup>f</sup>Centro de Investigaciones Económicas, Administrativas y Sociales, 120 Lauro Aguirre, Agricultura, Distrito Federal, 11360, Mexico.

**ABSTRACT**

Mexico City Metropolitan Area (MCMA) is the most populated urban area in the country. In 2010, MCMA required 14.8% of total energy domestic demand, but greenhouse gas emissions accounted for 7.7% of domestic emissions. Mexico has massive renewable energy potential that could be harnessed through solar photovoltaic (PV) technology. In that matter, marginalized population is severely affected by techno-environmental repercussions, therefore, there are several government policies within MCMA that focus on energy issues and social exclusion. The problem to explore is the relationship between local and federal public strategies in MCMA and their stance on energy transition concern, social empowerment, new technology appropriation and the will to boost social development and urban sustainability. A public policies typology was conducted through instruments of State intervention approach, based on political agenda articulation and environmental local interactions. In energy-environmental sector, six policies and seventeen instruments were identified and for social sector, three policies and ten instruments were detected. Social equality is encouraged by means of forthright funding and in-kind support and energy policies focus on non-renewable energy subsidies and electric transmission infrastructure investment. There is a lack of vision for using PV technology as guiding axis for marginalized population development. It is essential to promote economic and political rearrangement in order to level and structure environmental governance. Environmental networks consolidation must be achieved with participatory democracy and it is essential to understand people's representation about their own needs along with renewable energy.

**Keywords:** Photovoltaic technology, Social development, Environmental governance, Mexican policy

\* Corresponding author: Angel Raúl Arenas Aquino, +52 55 6131 0946, [rarenas@cinvestav.mx](mailto:rarenas@cinvestav.mx)



**Technical and economical feasibility analysis of biorefineries for  
hydrogen production**

**R. Cárdenas<sup>a,\*</sup>; D. Alfonso<sup>b</sup>; A. Pérez-Navarro<sup>b</sup>**

<sup>a</sup>Universidad Autónoma de Zacatecas – Unidad Académica de Ciencias Químicas, Edificio 6, Carretera Zacatecas - Guadalajara, La Escondida, 98160 Zacatecas, Zac.

<sup>b</sup>Universidad Politécnica de Valencia – Instituto de Ingeniería Energética, Camino de Vera s/n edificio 8e, cubo F 46022 Valencia, España.

**ABSTRACT**

The use of hydrogen as a fuel shows a growing interest driven by the increasing use of electric cars in developed countries. The use of renewable energies as a source of hydrogen is meant to play an important role in a future hydrogen economy, not only for being a clean source of it, but also for being a distributed source that is not restricted by political nor geographical issues, like fossil fuels are.

Biomass can become an important source of hydrogen either by thermochemical treatment or by biological fermentation. However, it is important to stress that not all biomass should be used. Second generation biofuels promote the use of non-food biomass in order to avoid the competition between energy needs and food needs, and helping to reuse non productive lands or agricultural residues as biomass feedstock.

This work aims to analyse the production of hydrogen by thermal gasification of biomass by modelling a biorefinery facility with different technologies from an economic and technical perspective. To do this, it was supposed the use of a mixture of agricultural residues from the Valencian Community in Spain.

The results showed that it was possible to model a biorefinery with an installed capacity of 310 MW<sub>th</sub>. The concept simulated using oxygen as a gasification agent presented the best energy efficiency with 53%, but also is more expensive than the concept using air gasification.

The size of the proposed facility is small in order to compete with the existing energy sources, but by increasing the plant size its economy improves. Furthermore, the use of political instruments to promote the zero carbon emissions energy sources and the production of nonfood feedstock can help to reduce the gap between biomass and fossil sources and make the biorefineries technologies more profitable.

**Keywords:** Hydrogen production, Biomass gasification, Hydrogen economy, Biorefineries

\* Corresponding author:

Rogelio Cárdenas Vargas, (+52 4921161450) rcardenasv@uaz.edu.mx

**Technical analysis and environmental gains of including biohydrogen in a conventional oil refinery**

**E. Mar-Juárez<sup>a</sup>; F. J. Ortega-García<sup>b</sup>**

<sup>a</sup>Instituto Mexicano del Petróleo, Gerencia de Transformación de la Biomasa, Eje Central Lázaro Cárdenas No152. México, D.F. CP 07730. MÉXICO. emar@imp.mx

<sup>b</sup> Gerencia de Servicios Químicos; Instituto Mexicano del Petróleo; Eje Central Lázaro Cárdenas No152. México, D.F. CP 07730. MÉXICO; fjortega@imp.mx

**ABSTRACT**

Hydrogen is fundamental for the modern oil refining industry as it is vastly used in hydrogenation processes like hydrodesulfurization or catalytic hydrocracking. The goal is to remove sulfur and nitrogen from the feedstocks by forming hydrogen sulfide and ammonia, thus making “cleaner” fuels.

Hydrogen is mainly produced in oil refineries via the catalytic reforming of light hydrocarbons with steam, typically using natural gas as a feedstock. Other technological options to produce Hydrogen are variations of the technology mentioned like partial oxidation of hydrocarbons and autothermal reforming.

In this paper, an alternative feedstock like biomass is technologically studied to produce part of the hydrogen needs of an oil refinery via its gasification and consequent reformation of this syngas. The biomass studied is wheat and sorghum husk which is cheaper than natural gas and has the clear advantage that its greenhouse gas emissions are practically zero. A life cycle evaluation is also carried out that clearly establishes that using biohydrogen in an oil refinery is feasible and very beneficial because it reduces the huge ecological footprint and is a concrete alternative in the short term because it uses infrastructure that is already there.

**Keywords:** Biohydrogen, Biomass, Refining, Renewable energy, Life cycle

\* Corresponding author:

F. J. Ortega-García, Gerencia de Servicios Químicos; Instituto Mexicano del Petróleo; Eje Central Lázaro Cárdenas No152. México, D.F. CP 07730, México; fjortega@imp.mx

## **Market research in Mexico of Hydrogen technologies**

**A.A. Hernández Bautista<sup>a,\*</sup>; J.M. Pineda Sandoval<sup>a</sup>; R. de G. González Huerta<sup>b</sup>**

<sup>a</sup>IPN-ESIME-Azc, SEPI, Av. De las Granjas, N°.682, Azcapotzalco. CP. 02250. México DF.

<sup>b</sup>ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPLAM, CP 07738, México, D.F

### **ABSTRACT**

Currently research about the use of hydrogen as fuel is extensive, however its participation in the energy system is low if it is compared with other alternative sources of energy (biofuel and biodiesel). According to the information obtained from hydrogen supply and demand, significant presence of hydrogen was found in some countries like USA, Japan and several European Union countries. In addition, some emerging applications are being developed in Brazil, Argentina, and Australia. Nevertheless, this information is not enough to make a projection of the supply and demand of using hydrogen in our country. This work highlights the importance of spreading the use of hydrogen in our society and also the result of a market research developed to know the feasibility of commercialization of hydrogen technology.

**Keywords:** Market research, Supply and demand, Hydrogen Technologies

\*Corresponding author:

Areli Anai Hernández Bautista; (55)49522435; E-mail: anaihb@hotmail.com

## **Nanostructured materials**



**Ionic and thermal conductivity of  $\text{Ln}_2\text{Hf}_2\text{O}_7$  hafnates (Ln=lanthanides)  
prepared by mechanical milling**

**F.A. López-Cota<sup>a</sup>; J.A. Díaz-Guillén<sup>b</sup>; O. J. Durá<sup>c</sup>; M. A. López de la Torre<sup>c</sup>;  
A.F. Fuentes<sup>a\*</sup>**

<sup>a</sup>Cinvestav Unidad Saltillo, Apartado Postal 663, 25000-Saltillo, Coahuila, Mexico.

<sup>b</sup>División de Estudios de Posgrado e Investigación, Instituto Tecnológico de Saltillo, 25280-Saltillo, Coahuila Mexico.

<sup>c</sup>CFMA, Departamento de Física Aplicada, Escuela Técnica Superior de Ingenieros Industriales, Universidad de Castilla-La Mancha, 13071-Ciudad Real, Spain.

**ABSTRACT**

Pyrochlore- and fluorite-type lanthanide hafnates with the general formula  $\text{Ln}_2\text{Hf}_2\text{O}_7$  (Ln = lanthanides and Y), belong to a group of mixed oxides with interesting electrical and thermal properties. Because of their high ionic conductivity, low thermal conductivity and high thermochemical stability, they might be considered promising electrolyte candidate materials for application in solid oxide fuel cells (SOFC's) and efficient thermal barrier coatings for protecting metallic components of gas turbines and diesel engines. Oxides properties are greatly affected by the presence of defects and disorder which occur easily in this particular group of hafnates; the density of defects in any particular sample is influenced by both, intrinsic (*e.g.*, chemical composition and cations size mismatch) and extrinsic factors (*e.g.*, thermal history and processing conditions). This contribution will analyze the influence of defects and disorder on the electrical and thermal properties of lanthanide hafnates  $\text{Ln}_2\text{Hf}_2\text{O}_7$ . Samples analyzed in this work were prepared at room-temperature, by mechanically milling stoichiometric mixtures of the corresponding elemental oxides. As reactants are processed under non-equilibrium conditions, mechanical milling offers the possibility of obtaining uncommon and highly defective metastable phases which are inaccessible for more conventional processing techniques. As-prepared samples were characterized by using XRD and Raman spectroscopy; irrespective of the lanthanide ion involved, they all consist of fluorite-like materials, although those containing  $\text{Sm}^{3+}$ ,  $\text{Eu}^{3+}$ , and  $\text{Gd}^{3+}$ , evolved into a pyrochlore structure, on heating. Electrical properties of sintered pellets were measured by using impedance spectroscopy, as a function of temperature and frequency. Thermophysical properties were measured by using differential scanning calorimetry (for the specific heat) and the laser flash method (thermal diffusivity). Experimental results compare favorably with those obtained for similar materials prepared by more complex processing techniques.

**Keywords:** Mechanical milling, Pyrochlore, Conductivity, Fluorite

\*Corresponding author: tel.: +52 844 4389617; email: fuentesaf@live.com



**Electrical properties of  $\text{Gd}_{1-x}\text{Ca}_x\text{Ti}_2\text{O}_{7-\delta}$  ionic conductors obtained by a novel ultrasound-assisted wet-chemistry method**

**M.R. Valdés-Ibarra<sup>a</sup>; K. P. Padmasree<sup>a</sup>; S. M. Montemayor<sup>b</sup>; J. A. Díaz-Guillén<sup>c</sup>;  
A.F. Fuentes<sup>a,\*</sup>**

<sup>a</sup> Cinvestav Unidad Saltillo, Apartado Postal 663, 25000-Saltillo, Coahuila, Mexico.

<sup>b</sup> Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna No. 140, 25294-Saltillo, Coahuila, Mexico.

<sup>c</sup> División de Estudios de Posgrado e Investigación, Instituto Tecnológico de Saltillo, 25280-Saltillo, Coahuila Mexico.

**ABSTRACT**

Lanthanide titanates  $\text{Ln}_2\text{Ti}_2\text{O}_7$  crystallizing with the pyrochlore structure, exhibit a wide range of physical and chemical properties of interest for both, fundamental science and practical applications. One of the most attractive features of these materials is that they can simultaneously support ionic and electronic charge carriers, which are required for mixed ionic-electronic conduction. Mixed conducting lanthanide titanates would allow the assembly of monolithic solid state electrochemical cells based on the pyrochlore structure. Such systems offer a significant advantage in terms of the mechanical, thermal and chemical stability over more heterogeneous devices. In particular, there is an important possibility of modulating the electrical properties of  $\text{Gd}_2\text{Ti}_2\text{O}_7$ -based solid solutions, between those typical of a solid electrolyte, and a mixed conductor with high levels of electronic and ionic conduction. The present contribution deals with the synthesis, structural characterization and electrical properties of Ca-doped  $\text{Gd}_2\text{Ti}_2\text{O}_7$ . Samples were prepared by a novel wet-chemistry method assisted by ultrasound. Appropriate amounts of titanium isopropoxide, and Gd and Ca nitrates were dissolved in a mixture of ethanol and ethylene glycol (volumetric ratio of 9:1) under vigorous magnetic stirring; the solution was then, irradiated for 1 h, aged and dried at 95°C to yield a gel, which was further processed at various temperatures and characterized by using different analytical techniques. Electrical properties of the as-prepared powders were measured as a function of temperature and frequency by using impedance spectroscopy and pellets sintered at 1200 and 1500°C. Ca-doped  $\text{Gd}_2\text{Ti}_2\text{O}_7$  samples show impedance spectra similar to those typical of most solid electrolyte materials; whereas, log-log representations of the frequency dependence of the real part of the electrical conductivity at different temperatures, are in agreement with the so-called “Universal Dielectric Response” (UDR) proposed by A.K. Jonscher. The complex impedance plots Arrhenius plots confirm that the *dc* conductivity is thermally activated with activation energies within the 0.7-0.9 eV range, depending on Ca-content and sintering temperature.

**Keywords:** Gadolinium titanate; Ionic conductivity; Ultrasound; Impedance spectroscopy

\* Corresponding author: tel.: +52 844 4389617; email: fuentesaf@live.com

**Electrocatalytic oxygen evolution reaction in alkaline media using a hydrotalcite-like material Ni/Co-Fe**

**J. Vazquez-Samperio<sup>a,b</sup>; M.A. Oliver-Tolentino<sup>b</sup>; A. Diaz-Romero<sup>a</sup>;  
A. Guzman-Vargas<sup>b</sup>; E. Reguera-Ruiz<sup>a</sup>**

<sup>a</sup>Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada del Instituto Politécnico Nacional, Legaria 694. Colonia Irrigación, 11500 México D. F.

<sup>b</sup>ESIQIE-IPN, Laboratorio de Investigación en Materiales Porosos Catálisis Ambiental y Química Fina, UPALM Edif. 7 P.B. Zacatenco México D.F. 07738, Mexico.

**ABSTRACT**

High activity, durable, and cost effective electrocatalyst for the oxygen evolution reaction (OER) plays an important role in electrochemical science and technology, for example, water-splitting by electrolysis for production of hydrogen. The first-row transition-metal-based OER catalysts, especially iron-, cobalt- and nickel-containing materials, are versatile candidates for replacement of precious catalysts due to their earth abundant nature, low cost, environmentally friendly, multiple valence state and high theoretical activity. In this study we reported the oxygen evolution reaction (OER) using a new and efficient hydrotalcite-like (LDH) material Ni/Co-Fe.

The LDH's Ni/Co-Fe was synthesized by co-precipitation method at varied Ni/Co ratios (e.g. 1:1 (#1), 2:3 (#2), and 3:2 (#3)) keeping constant Ni/Co-Fe ratios (e.g. 2:1). The materials were characterized by X-Ray Diffraction, Infrared Spectroscopy, showed that the hydrotalcite structure was obtained. Then, Static magnetic measurements were performed in a superconducting quantum interference device (SQUID) with freshly prepared powdered samples. As previously reported for several magnetic LDHs, Ni/Co-Fe LDHs are ferrimagnets due to the coexistence of ferromagnetic Ni-OH-Ni, Ni-OH-Co or Co-OH-Co superexchange interactions and antiferromagnetic Co-OH-Fe, Fe-OH-Fe, Ni-OH-Fe or Ni-OH-Co interactions mediated by the -OH bridges. At room temperature, all samples are attracted by a conventional laboratory magnet. The behaviour in the Ni/Co-Fe-LDH's is probably related to a superparamagnetic effect. The cyclic voltammetry experiments showed that OER starts c.a. 0.43 V, where the LDH Ni/Co-Fe #2 presented a higher catalytic activity. This catalytic activity is discussed due to the effect of magnetic behavior in LDH's.

In summary, HDL's have been obtained by co-precipitation; HDL's have been structurally characterized by XRD, IR Spectroscopy, SQUID and their properties have been studied by voltammetric techniques. The HDL's present superparamagnetic effect. The LDH Ni/Co-Fe (2:3 Ni:Co) exhibited the better catalytic activity.

**Keywords:** Water electrolysis, Hydrotalcite, Superparamagnetic, Ferrimagnets

\* Corresponding author:

M.A. Oliver-Tolentino, otma\_iq@hotmail.com



**Insertion/Desertion of  $\text{Na}^+$  and  $\text{Mg}^{2+}$  in Cobalt Hexacyanoferrate towards electrochemical energy storage**

**M. A. Oliver Tolentino<sup>a,b</sup>; D. Rodríguez-Morán<sup>c</sup>; B. Tapia-Juarez<sup>c</sup>;  
A. Guzmán-Vargas<sup>c</sup>; E. Reguera<sup>a</sup>**

<sup>a</sup> Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Legaria 694. Col. Irrigación, México D. F., C.P.: 11500.

<sup>b</sup> Departamento de Bioingeniería, UPIBI-IPN, Av. Acueducto de Guadalupe S/N, Gustavo A Madero, Barrio La Laguna Ticoman, 07340 Ciudad de México, D.F.

<sup>c</sup> Laboratorio de Investigación en Materiales Porosos, Catalisis Ambiental y Química Fina, ESIQIE-IPN, UPLM, Gustavo A. Madero, Ciudad de México, D.F.

**ABSTRACT**

Recently, battery research has focused on the high power and energy density needed for portable electronics. However, the requirements for grid-scale energy-storage are different, with emphasis on low-cost production. In this context the use of  $\text{Mg}^{2+}$  and  $\text{Na}^+$  in aqueous ion batteries has been an encouraging promise, due to the abundance of these alkaline ions in the planet. On the otherhand, open framework materials with the Prussian Blue crystal structure (PBAs) offer high power capabilities and low-cost synthesis. In this contribution the  $\text{KCo}[\text{Fe}^{\text{III}}(\text{CN})_6]$  was synthesized; the Co-HCF was mixed with amorphous carbon, polyvinylidenedifluoride, and graphite. The obtained suspension was deposited on a glassy carbon electrode; the experiments were carried out in a  $\text{NaNO}_3$  and  $\text{MgNO}_3$ . The galvanostatic experiments shows a high stability for charge-discharge (>100 cycles) with a reversible capacity of  $116.8 \text{ mAhg}^{-1}$  at 0.83C in presence of both Ion. This capacity is associated to redox process of  $\text{Co}^{\text{III}}/\text{Co}^{\text{II}}$  and  $\text{Fe}^{\text{III}}/\text{Fe}^{\text{II}}$  site, however the electrochemical mechanisms during charge-discharge process is different provokes that the charge retention to different rate enhance in  $\text{Mg}^+$  ion batteries; this behavior is discussed based on the insertion and removal of ions and of their location within the cavities of the structure during the charge and discharge cycles.

**Keywords:** Insertion-Desertion, Open framework, Ion Batteries, Charge retention

\* Corresponding author:  
Miguel Angel Oliver Tolentino, otma\_iq@hotmail.com

**Kinetic study of Ptx/Moy/CNT electrocatalyst in oxygen reduction reaction**

**S. Montoya Solís<sup>a,b</sup>; R. de G. González Huerta<sup>a\*</sup>; M. Beltrán Villavicencio<sup>b</sup>;  
E. Torres Santillán<sup>a</sup>**

<sup>a</sup>ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, UPALM, C.P. 07738, México D.F.

<sup>b</sup>UAM-Azc, CBI, Av. San Pablo, No.180, C.P. 02200, México D.F.

**ABSTRACT**

The kinetics of the ORR of Ptx/Moy/CNT (x=10,8,5,2 and y=0,2,5,8) nanoparticles were studied in acid media. The carbon nanotubes (Sigma-Aldrich 97%) were treated by an oxidation method in nitric acid aqueous solution (functionalization process). The electrocatalysts were synthesized by chemical reduction of the metal acetylacetonate (Pt and Mo) with NaBH<sub>4</sub> in methanol media. Materials were characterized structurally and morphologically by X-ray diffraction, scanning electron microscopy and transmission electron microscopy. Electrochemical studies were performed by cyclic voltammetry and rotating disk electrode (RDE) techniques. Kinetic parameters exhibited Tafel slopes between 90 and 120 mV dec<sup>-1</sup> and exchange current density of around  $1 \times 10^{-5}$  mAcm<sup>-2</sup>. A four-electron reduction was found in all cases. The best catalyst was 8% Pt 2% Mo/ NTC. The enhanced reactivity of the catalysts surfaces is attributed to their electronic and geometric structure associated to the bifunctional effects, in which the unique catalytic properties of each of the elements in the catalytic compound combine in a synergetic manner to yield a surface which results more active than each of the elements alone. Authors thank CONACYT to the Programa de Redes Temáticas (RTH2) projects 252003 and 249795; and IPN SIP multidisciplinary project 1683.

**Keywords:** Oxygen reduction reaction, Nanomaterials PtxMoy/CNT, Electrocatalyst

\* Corresponding author:

Rosa de Guadalupe González Huerta, (+52) 55 57296000 ext 54246, rosgonzalez\_h@yahoo.com.mx

**Efficient photoreforming of glycerol on Ag/TiO<sub>2</sub>/ZSM-5  
composites under UV and visible light**

**N. Pineda <sup>a</sup>; M. A. Valenzuela <sup>a,\*</sup>; S. Alfaro <sup>a</sup>; F. M. Martínez <sup>a</sup>**

<sup>a</sup>Lab. Catálisis y Materiales. ESIQIE-Instituto Politécnico Nacional. Zacatenco, 07738, México D.F.

**ABSTRACT**

TiO<sub>2</sub>/ZSM-5 composites were synthesized by a solvothermal method employing titanium propoxide, ethanol as solvent in acetic acid solution, CTAB as surfactant and commercial ZSM-5 zeolite. Subsequently, silver nanoparticles were selectively photo-deposited on the TiO<sub>2</sub>/ZSM-5 composites by using an alcoholic solution of silver nitrate under UV-light (365 nm). The as-prepared photocatalysts were characterized by X-ray diffraction, nitrogen physisorption, diffuse reflectance spectroscopy, infrared spectroscopy, scanning/transmission electron microscopy and time-resolved microwave spectroscopy. The photocatalytic properties of the Ag/TiO<sub>2</sub>/ZSM-5 composites were studied for the glycerol photoreforming in aqueous suspensions under UV and visible irradiation. According to the results, TiO<sub>2</sub> (anatase) was homogeneously distributed among the bulk and surface of zeolite and decorated with Ag nanoparticles. There was no chemical interaction between TiO<sub>2</sub> and zeolite, which means that this last compound was only a support of the semiconductor. Silver addition (1 wt.%) caused a significant reduction of the band gap of TiO<sub>2</sub>, from 3.0 to 2.1 eV, showing a surface plasmon resonance effect at around 400 nm. The modification of TiO<sub>2</sub> and TiO<sub>2</sub>/ZSM-5 composites with Ag nanoparticles induced an increase in the photocatalytic activity under both UV and visible light. These results were explained in terms of a decrease of charge-carrier recombination under UV-light and electron injection from Ag nanoparticles to TiO<sub>2</sub> under visible light.

**Keywords:** Photocatalysis, Glycerol photoreforming, Ag/TiO<sub>2</sub>/ZSM-5

\* Corresponding author:

Miguel A. Valenzuela, Phone: 5255-57296000-55112, Fax: 5255-55862728, Email: mavalenz@ipn.mx



**Polyaniline films fabricated by electrochemical polymerization: A systematic electrochemical study**

**O. Martínez-Alvarez<sup>a,\*</sup>; C. J. Yerena-Moreno<sup>a</sup>; M. C. Arenas-Arrocena<sup>b</sup>;  
B. Ruiz-Camacho<sup>c</sup>; A. S. Ordeñana-Martínez<sup>a</sup>**

<sup>a</sup>Ingeniería en Energía, Universidad Politécnica de Guanajuato, Av. Universidad Norte s/n, Juan Alonso Cortázar Guanajuato, 38483, México.

<sup>b</sup>Escuela Nacional de Estudios Superiores, Unidad León, UNAM, México, Boulevard UNAM No. 2011 predio el Saucillo y el potrero C.P. 36969, León Guanajuato México.

<sup>c</sup>Departamento de Ingeniería Química, Universidad de Guanajuato, División de Ciencias Naturales y Exactas, Noria Alta s/n, Col. Noria Alta, Guanajuato, Gto, 36050, México.

**ABSTRACT**

Conducting polymers are modern materials with various applications whose synthesis and properties have been studied extensively due to the growing interest in the mechanism of their polymerization and redox transformation between conductive and pasive states, the polyaniline (Pani) is one of the most potential conducting polymers due to its various potential application suchs as batteries, electrochemical capacitors, dye-sensitized solar cell, electrochromic and electroluminescent devices.

In this study, polyaniline films were fabricated on stainless steel 304 substrate(SS) trough different electrochemical techniques cyclic voltammetry, Chronopotentiometry and Chronoamperometry, from 1M H<sub>2</sub>SO<sub>4</sub> solution containing 0.1M, 0.2M and 0.3M of aniline. The cyclic voltammograms show peaks anodic/cathodic associated at the different stages of growth and its correlation with oxidation states de Pani, the analysis of potential and peak currents shows small differences in the concentrations tested. The obtained Pani films differs in its oxidized states, wich results in morphological and structural differences of Pani deposits on SS due to hydrolysis reactions.

**Keywords:** Polyaniline films, Cyclic Voltammetry, Pani morphology

\* Corresponding author:

Omar Martínez Alvarez, +524614414300 ext. 4317, [omartinez@upgto.edu.mx](mailto:omartinez@upgto.edu.mx)



**Impedance study of the electrocatalytic reduction of oxygen on  
Pt/C and Pt-Ag/C**

**B. Ruiz Camacho<sup>a,\*</sup>; E. Romero Mendoza<sup>b</sup>; J.C. Baltazar Vera<sup>a</sup>; R. Fuentes Ramírez<sup>a</sup>;  
O. Martínez Alvarez<sup>b</sup>**

<sup>a</sup>Departamento de Ingeniería Química, Universidad de Guanajuato, División de Ciencias Naturales y Exactas, Noria Alta s/n, Col. Noria Alta, Guanajuato, Gto, 36050, México

<sup>b</sup>Ingeniería en Energía, Universidad Politécnica de Guanajuato, Av. Universidad Norte s/n, Juan Alonso Cortázar Guanajuato, 38483, México

**ABSTRACT**

Nanoparticles of Pt and Pt-Ag were synthesized using sonication at room temperature with no consecutive thermal treatment to catalyze the acid oxygen reduction reaction (ORR) at room temperature. The metal nanoparticles obtained were supported on carbon Vulcan substrate. The electrochemical impedance spectroscopy (EIS) at different potentials was used for study the mechanism reaction and the kinetic of ORR on Pt and Pt-Ag nanosized electrodes in acid electrolyte. The physical properties, morphology and crystallinity of the electrocatalysts synthesized were investigated by X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM) analysis. The kinetic of the silver and platinum nanoparticles in solution was followed using UV-vis spectroscopy. The ORR was analyzed in acid medium at room temperature. Both materials synthesized shows a nanoparticle size of < 10 nm, however the Pt/C monometallic sample exhibit more significative aggregation than Pt-Ag/C catalyst. Pt-Ag/C exhibit better electrochemical properties to catalyze the ORR compare to Pt/C. The analysis of the impedance diagrams of both materials tested revealed at least the presence of two-electron reaction process involved in the reduction reaction depending of the potential applied.

**Keywords:** EIS, Ultrasound, Oxygen reduction, Platinum, Silver

\* Corresponding author:

Beatriz Ruiz Camacho, +524737320006 ext. 8115, beatrizruizcamacho@gmail.com

**Selective heterogeneous nucleation of Platinum nanoparticles onto graphitic domains of multi-walled carbon nanotubes**

**C.A.Campos-Roldán<sup>1,2,3</sup>; R.G. González-Huerta<sup>1\*</sup>; J.R. Vargas-García<sup>2</sup>;  
N. Alonso-Vante<sup>3</sup>**

<sup>1</sup>ESIQIE-IPN Laboratorio de electroquímica y corrosión, UPALM 07738, México D.F., México

<sup>2</sup>Depto. Ing. Metalúrgia y Materiales, Instituto Politécnico Nacional, México 07300 D.F., México

<sup>3</sup>IC2MP, UMR-CNRS 7285, University of Poitiers, 4 rue Michel Brunet, 86022 Poitiers, France

**ABSTRACT**

The strong interaction between extended graphitic domains of multi-walled carbon nanotubes (MWCNTs) and platinum nanoparticles (Pt NP's) was investigated. Three different chemical treatments were performed on pristine home-made MWCNT to modify the graphitic domains, as revealed by Raman spectroscopy, whose analyses indicated the development of  $sp^2$  character. The integrated G band intensity becomes higher and narrower than the integrated D band intensity.

Pt NP's were photo-deposited using UV-VIS light onto modified MWCNTs. The effect of the strong interaction on the electronic properties of Pt NP's was electrochemically probed by CO stripping. We can appreciate the CO oxidation multi-peak signals. A correlation between the in-plane crystallite size ( $L_a$ ) of the carbon supports, and the oxidation charge of CO stripping experiments was made. Analyses of the CO oxidation revealed the presence of two peaks centered at 0.63V and 0.66V. We found that 80% of the electrochemical active surface area (*ECSA*) of the photo-deposited electrocatalyst correlates well with the highest  $L_a$  and belongs to the peak centered at 0.63V, whereas this parameter at the same electrode potential decreases as  $L_a$  decreases. Parallel with that observation, *ECSA* at 0.66V increases as the support possesses a high  $sp^3$  character. This interaction results from the heterogeneous nucleation of Pt NP's onto the carbon support domains. It appears that  $\pi$ -system of graphitized carbon anchors Pt NP's in a way that strongly modifies the electronic properties of the Pt valence band.

The authors thank CONACYT to the Programa de Redes Temáticas (RTH2) projects 252003 and 249795; and IPN SIP projects 1683 and 20151824.

**Keywords:** Carbon Nanotubes, Pt nanoparticles, CO oxidation, Oxygen Reduction Reaction

\* Corresponding author:

Rosa de Guadalupe González Huerta, (+52) 55 57296000 ext 54246, rosgonzalez\_h@yahoo.com.mx

**Synthesis and characterization of carbon nanofibers for  
fuel cell applications**

**R. Ojeda-López<sup>a</sup>; G. Ramos-Sánchez<sup>a,b\*</sup>; J.G. Vazquez-Arenas<sup>a</sup>;  
J.M. Esparza-Schulz<sup>a</sup>; A. Dominguez-Ortíz<sup>a</sup>; I. González<sup>a</sup>**

<sup>a</sup>Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, Col. Vicentina, 09340 Mexico City, Mexico.

<sup>b</sup>Cátedras CONACYT comisionado a Universidad Autónoma Metropolitana.

**ABSTRACT**

Carbon nanofibers (CNFs) are materials with potential applications as electrode supports in fuel cells, mainly due to their interesting characteristics: i) high surface area, ii) controlled chemical properties, and iii) high electric conductivity. Enhanced interaction between the support and the active material is supposed to improve the catalyst dispersion and increase the resistance to agglomeration. CNFs can be prepared by nitrogen doping, this procedure allows the formation of specific sites on the nanofibers surface which lead to controlled size and dispersion of the active material.

In this work, polyacrylonitrile nanofibers (PAN) are synthesized by electrospinning, then CNFs are obtained by PAN carbonization. The properties of CNFs are controlled by the calcination conditions, two heat treatments make up the calcination process: i) stabilization under oxidizing atmosphere, and ii) carbonization under inert atmosphere. On the first process the fibers are treated at 543 K in order to promote cyclization and partial dehydrogenation, this process helps to keep the fibrous structure of system. On the second treatment CNFs are obtained by heating beyond 973 K, in this stage carbon content grows, and depending on the temperature varying ratios of amorphous and crystalline phases are formed. When the carbonization temperature increases, nitrogen and hydrogen concentrations decrease, but carbon array crystallinity rises. With the idea of prepare the best nanofibers to fuel cell operation, four different carbonization temperatures (973, 1073, 1173 and 1273 K) are explored. The electrochemical characterization indicates that all CNFs present a more positive oxidation potential in comparison to carbon Vulcan. This result is in agreement with thermogravimetric analysis in which CNF decomposition (CO<sub>2</sub> formation) is obtained at higher temperatures in comparison to commercial supports. Preliminary results indicate that the lower the calcination temperature the higher amount of N groups leading to improved interaction Pt nanoparticles – support.

**Keywords:** Fuel cell, CNF's, PAN, Catalyst support

\*G. Ramos-Sánchez, +52 55 5804 4600 ext 4396, gramossa@conacyt.mx

**Preparation of electrospun SPEEK-PVB nanofiber embedded in  
SPEEK-PVA blend as composite membrane for PEM fuel cells**

**J.L. Reyes-Rodríguez<sup>a</sup>; E. Giménez<sup>b</sup>; O. Sahuquillo<sup>b</sup>; A. García<sup>b</sup>;  
O. Solorza-Feria<sup>a</sup>; V. Compañ-Moreno<sup>b\*</sup>**

<sup>a</sup>Departamento de Química - Centro de Investigación y de Estudios Avanzados del I.P.N., Av. IPN 2508, Col. San Pedro Zacatenco, 07360 México D.F., México.

<sup>b</sup>Escuela Técnica Superior de Ingenieros Industriales - Universidad Politécnica de Valencia, Camino de vera s/n, 46020 Valencia, España.

**ABSTRACT**

Proton exchange membrane (PEM) plays an important role in the ionic transport process from the anode to the cathode in a protonic exchange membrane fuel cell (PEMFC). Actually, Nafion<sup>®</sup> membranes are the most used due to its high protonic conductivity. However Nafion<sup>®</sup> only can be used efficiently at operating temperature below from 80°C because above of these conditions is dehydrated and significantly decreases its ion exchange capacity, besides presenting stability problems too. Sulfonated Polyether ether ketone (SPEEK) is a potential candidate to replace Nafion<sup>®</sup> membranes due to its glass transition temperature is above 170°C, therefore would be possible to operate fuel cells at intermediate temperature (120-140°C). In recent years the development of composite polymeric membranes obtained by electrospinning for use in PEMFC has gained significant interest due to their attractive features such as good chemical and physical properties, efficiency, strength, durability, low production costs, among others. In the present work, SPEEK<sub>70wt%</sub>-PVB<sub>30wt%</sub> (PVB - Polyvinyl butyral) based composite nanofibers were prepared by varying the electrospinning time in order to obtain mats with different thickness. The mats were embedded in a SPEEK<sub>65wt%</sub>-PVA<sub>35wt%</sub> (PVA - Polyvinyl alcohol) polymer solution to fill the pores of the fiber. The membranes obtained were characterized by Scanning Electron Microscopy (SEM) where was possible to observe the fibers embedded appropriately in the SPEEK-PVA polymer matrix. Microtensile test revealed that the maximum tensile strength increases as the thickness of the SPEEK-PVB nanofiber mat increases too, making more flexible composite membranes respect to a SPEEK-PVA pure membrane obtained by casting. Impedance spectroscopy allowed to obtain the protonic conductivity of the membranes. The best conductivity (0.038 S cm<sup>-1</sup>) was obtained at 120°C for the composite membrane with a SPEEK-PVB nanofiber mat of 12 h of electrospinning time. While this conductivity is low compared to Nafion (0.083 S cm<sup>-1</sup>) it is truly remarkable that these membranes are attractive because they allow to work in a temperature range higher than the commercial Nafion without losing its strength or its hydration capacity, improving thus proton conductivity. That make them potential candidates for fuel cells.

**Keywords:** SPEEK membranes, Composite membranes, Electrospinning, PEMFC membranes

\* Corresponding author:

Vicente Compañ-Moreno, Tel.: +34 96 387 9328; fax: +34 96 387 7924, vicommo@ter.upv.es

**Biosynthesis of iron nanoparticles for perchloroethylene treatment**

**L. Bretón-Deval; H. M. Poggi-Varaldo\* ; E. Ríos-Leal; O. Solorza-Feria**

Environmental Biotechnology and Renewable Energies R&D Group, Dept. Biotechnology & Bioengineering, CINVESTAV- I.P.N. Av. Instituto Politécnico Nacional 2508, CP 07360, Mexico D.F.

**ABSTRACT**

Several works have been carried out with the aim of removing perchloroethylene (*PCE*) and metabolites using iron nanoparticles (*NPs*) because iron can serve as a fixed source of electrons for the reductive dehalogenation of *PCE*. However these *NPs* could be very reactive; they quickly oxidize and lose their reductive power. Some research has focused on the synthesis of *NPs* using specific microbes. However, so far, this technique also known as biosynthesis of *NPs* has not used a dehalogenating consortium as a driving agent. We hypothesized that the *in situ* biosynthesis of iron *NPs* by the consortium would allow a prompt use of the *NPs* for effective dehalogenation of *PCE*. Therefore, the purposes of this research were (i) to biosynthesize active iron *NPs* using a dehalogenating consortium, and (ii) to evaluate the removal/degradation of *PCE* by these *NPs*.

A batch experiment was implemented in order to test two different types of precursor iron salts. The batch units were loaded with 5 g/L of dehalogenating consortium, plus 6 g/L methanol, and precursor salts, either  $\text{FeCl}_3$  or  $\text{Fe}(\text{NO}_3)_3$ . For the degradation tests, *PCE* was added at an initial concentration of 80 mg/L.

The consortium could successfully use both types of salts for synthesizing iron *NPs*. The average diameter of *NPs* was around 5 nm; yet, aggregates 30 – 70 nm diameter were also found. Samples from the treatment that used the  $\text{Fe}(\text{NO}_3)_3$  showed more aggregates while the other treatment showed smaller *NPs*. The removal of *PCE* was more efficient in the treatment of *PCE* with the chloride salt, after 4 days the removal was 99%. The *NPs* biosynthesized with  $\text{Fe}(\text{NO}_3)_3$  removed only 78% of *PCE*. On the other hand, the control units containing dehalogenating consortium but no *NPs* could just remove 15%. In general, the main *PCE* metabolite found was *TCE*. We conclude that the dehalogenating consortium is capable of synthesizing *NPs* that can effectively degrade *PCE*, second, the *NPs* obtained from  $\text{FeCl}_3$  precursor exhibited smaller diameter and increased rates and extents of pollutant removal. Finally, our biosynthesis route for iron *NPs* implies significant savings in chemical reagents as well as energy in contrast to the typical chemical techniques for iron *NPs* fabrication

**Keywords:** Biosynthesis, Iron nanoparticles, *PCE* treatment, Water pollution

\* Corresponding author: Professor Dr. Héctor Mario Poggi-Varaldo, Environmental Biotechnology and Renewable Energies R&D Group, Dept. Biotechnology & Bioengineering, CINVESTAV- I.P.N. P.O. Box 14-740, 07000, México D.F., México  
Tel: 5255 5747 3800 x 4324. Fax : 5255 5747 3313, E-mail: r4cepe@yahoo.com

**Comparative electrocatalytic study of  $\text{Fe}_3\text{O}_4@\text{Pt}/\text{C}$  and  $\text{Fe}_2\text{O}_3@\text{Pt}/\text{C}$  core-shell nanostructures for the ORR**

**N. M. Sánchez-Padilla<sup>a</sup>; S. M. Montemayor<sup>b</sup>; F.J. Rodríguez-Varela<sup>a,c,\*</sup>**

<sup>a</sup>Programa de Sustentabilidad en Recursos Naturales y Energía, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, C.P 25900, Coahuila, México.

<sup>b</sup>Centro de Investigación en Química Aplicada, Blvd. Enrique Reyna No. 140, Col. San José de los Cerritos, 25294 Saltillo, Coahuila, México.

<sup>c</sup>Programa de Nanociencias y Nanotecnología, Av. Industria Metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, C.P 25900, Coahuila, México.

**ABSTRACT**

In this work, a comparative study of the catalytic activity for the Oxygen Reduction Reaction (ORR) of the core-shell structures  $\text{Fe}_3\text{O}_4@\text{Pt}/\text{C}$  and  $\text{Fe}_2\text{O}_3@\text{Pt}/\text{C}$  is presented. The a two-step route was followed to obtain the materials. First, the cores were obtained via a modified co-precipitation method using etilenglicol (EG) as a surfactant. In a second step, the deposition of the Pt shell was made via impregnation-reduction, using  $\text{NaBH}_4$  as reducing agent. The crystalline structure of the catalysts has been confirmed by XRD, showing the presence of the cubic inverse spinel phases of  $\text{Fe}_3\text{O}_4$  or  $\text{Fe}_2\text{O}_3$ . The patterns showed also the reflectios of fcc Pt, having particle size below 5 nm. The electrochemical measurements were carried out in 0.5 M  $\text{H}_2\text{SO}_4$  and 0.5 M KOH. The  $\text{Fe}_3\text{O}_4@\text{Pt}/\text{C}$  cathode delivered higher current density and showed higher degree of tolerance to ethanol than  $\text{Fe}_2\text{O}_3@\text{Pt}/\text{C}$ . On the other hand, both core-shell cathodes demonstrated enhanced tolerance properties related to a Pt/C cathode. Such characteristic has been attributed to the core-shell structure that modified the surface properties of Pt and also to the oxidation states of the iron oxide cores.

**Keywords:** Catalysts synthesis, Core-shell nanostructures, Oxygen reduction reaction

\* Corresponding author:

F.J. Rodríguez Varela, 52 +844 438-9600 (Ext. 8526), 25900, javier.varela@cinvestav.edu.mx



**Effect of change in shape of electrocatalysts core-shell Au-Pd in the oxygen reduction reaction**

**A. Romero-Hernández<sup>a</sup>; E. M. Arce-Estrada<sup>a,\*</sup>; M. E. Manríquez<sup>b</sup>;  
J.V. Medina-Flores<sup>a</sup>**

<sup>a</sup>Departamento de Ingeniería en Metalurgia y Materiales, Escuela Superior de Ingeniería Química e Industrias Extractivas, ESIQIE-IPN, México, D.F., 07738

<sup>b</sup>Laboratorio de Investigación en Físicoquímica y Materiales, Escuela Superior de Ingeniería Química e Industrias Extractivas, Instituto Politécnico Nacional, Edif. Z, sección 5, 2do Piso, México, D.F., 07738

**ABSTRACT**

The reduction reaction of oxygen is one of the reactions that takes place in a PEMFC and contributes largely to their good or bad performance. For this reason the use of Pt/C was the best option so far for cells with optimal performance, but its high cost has limited its use. It is noteworthy that platinum has not necessarily shown the best electrocatalytic activity since it is susceptible to contamination of the active sites, so the kinetics are slow over time. Recent studies have focused on the use of core-shell nanoparticles to use as electrocatalyst. Diverse Core-Shell structures have been developed as Pd-Pt with tetrapod morphology; this material had less overpotential than Pt/C. Also, this study demonstrated that the most active metal place for ORR on the surface (Core) and less active in the nucleus (Shell) increases electrocatalyst performance. Currently, there are few studies of Core-Shell nanoparticles with different shapes for use as electrocatalysts for the ORR in acid medium, so there are not advances in studies about efficient, performance and stability in the PEMFC. This work proposes synthesize, characterize and evaluate heterostructures Core-Shell Au-Pd, as electrocatalysts for the ORR. The Core-Shell Au-Pd nanoparticles were obtained by chemical synthesis and supported in Vulcan Carbon to evaluate its activity in the ORR. The heterostructures Core-Shell Au-Pd: octahedral, cubic concave and cuboctahedral were synthesized and characterized for XRD, SEM and TEM. The results indicate that the different Au-Pd shapes synthesized exhibit the core-shell nanostructure. Also the nanoparticles have shown a uniform particle size of about 50 nm for Pd shell and 20 nm Au cores as well as a difference between the shapes of the nanoparticles. XRD studies show characteristic peaks which presents Au due to low intensities found in the core of the nanoparticles. The ORR electrocatalyst were studied by electrochemical measurements. The core-shell nanostructures showed attractive catalytic activity with differences relating to the changing shape of the nanoparticles.

**Keywords:** Core-shell, Nanomaterials, ORR, PEMFC

\* Corresponding author:

Dr. Elsa Miriam Arce Estrada, Tel. 5557296000 Ext. 54212, Email: earce@ipn.mx





**Preparation and electrochemical study of M:TiO<sub>2</sub> (M= Sn, Ta, V) as support of IrO<sub>2</sub> for oxygen evolution reaction**

**J. Aldaba; M. Galvan-Valencia; I.L. Escalante-García; S.M. Durón-Torres\***

Universidad Autónoma de Zacatecas Unidad Académica de Ciencias Químicas, Campus Siglo XXI, Carretera Zacatecas-Guadalajara Km. 6.0, Ejido la Escondida, Zacatecas, Zacatecas, 98160, MÉXICO.

**ABSTRACT**

Titanium dioxide powder modified with tin, tantalum and vanadium at different atomic percentages was synthesized using the sol-gel method. The material obtained was characterized electrochemically by cyclic voltammetry (CV), linear sweep voltammetry (LVS), electrochemical impedance spectroscopy (EIS) and chronoamperometry (CA). The synthesized material was compared to TiO<sub>2</sub> anatase phase. To evaluate their performance as support for oxygen evolution reaction (OER), the synthesized oxides were decorated with IrO<sub>2</sub> as electrocatalyst. The data obtained during the OER were compared with those obtained for the same catalyst supported on Vulcan XC-72. The best support materials were those synthesized with vanadium and tantalum as a dopant. The results indicate that OER onset potential was increase approximately 60 mV with respect to that observed for Vulcan as support. The chronoamperometry results showed that the support material presents good stability for OER during 8 h. The preliminary results indicate that the modified titanium dioxide prepared could be used as anodic support in proton exchange membrane water electrolyzers.

**Keywords:** Nanomaterials, Oxygen evolution reaction, Sol-gel method, PEM water electrolyzer

\* Corresponding author:

Sergio Miguel Duron Torres, 52 492-925-6690 ext 4655, serduro@yahoo.com.mx

**Physicochemical and stability study of Ir-Sn-Sb-O materials as catalyst-supports for the oxygen evolution reaction**

**N. J. Pérez-Viramontes<sup>a</sup>; I. L. Escalante-García; C. Guzmán<sup>a</sup>; M. Galván-Valencia<sup>a</sup>;  
S. M. Durón-Torres<sup>a\*</sup>**

<sup>a</sup>Unidad Académica de Ciencias Químicas, Universidad Autónoma de Zacatecas, Campus Siglo XXI, Carretera Zacatecas-Guadalajara Km. 6.0, Ejido la Escondida, Zacatecas, Zacatecas, México, 98160.

**ABSTRACT**

A mixed oxide powder material, with general formula Ir-Sn-Sb-O, was prepared in one-step synthesis by the thermal decomposition of the chloride precursors  $\text{H}_2\text{IrCl}_6$ ,  $\text{SnCl}_4 \cdot 5\text{H}_2\text{O}$ , and  $\text{SbCl}_3$  in ethanol. This powder material is both an electrocatalyst and support for its possible use as anode in solid polymer electrolyte water electrolyzers (SPEWEs). Two theoretical atomic percent of iridium (10 and 40 at. % Ir) in the reaction mixture were considered to investigate the electrocatalytic activity of the mixed oxides toward the oxygen evolution reaction (OER) in acidic media. Preliminary results show that the mixed oxide material exhibited micrometric agglomerations of finer globular structures as observed from scanning electron micrographs (SEM). Additionally, the atomic composition of iridium was estimated to be near to the theoretical atomic percentages in the synthesis step for both mixed oxides materials, 10.7 at. % Ir for Ir-Sn-Sb-O (10) and, 45.0 at. % Ir for Ir-Sn-Sb-O (40) using energy dispersive X-ray analysis (EDAX) coupled to SEM. The present phases of the powder material and the particle size was analyzed by X-ray diffraction (XRD). The results indicated the presence of the iridium oxide, antimony oxide and metallic iridium in both materials. Overall, the particle size was estimated between 1 – 2 nm. The stability of the materials was evaluated by chronoamperometry (CA) at a potential of 1.55 V vs NHE during a period of 8 h, showing that the materials are stable. The conductivity of the mixed oxides was measured by four-probe method, the conductivity of both materials are greater than  $\text{SnO}_2$  and  $\text{Sb-SnO}_2$ . The results demonstrate a nanometric particle size with high stability for OER, thus the synthesized materials are suitable for their use as catalyst-support anode for PEM water electrolyzers.

**Keywords:** Iridium catalyst, Oxygen evolution reaction, Water electrolysis

\*Corresponding author:

Dr. Sergio M. Durón Torres, Tel: +524929256690 Ext. 4655; e-mail: [durosm@prodigy.net.mx](mailto:durosm@prodigy.net.mx)



**Defects and disorder in the  $\text{Gd}_2\text{Hf}_{2-x}\text{Zr}_x\text{O}_7$  solid solution:  
mechanochemical synthesis, characterization and electrical properties**

**N. M. Cepeda-Sánchez<sup>a</sup>; J. A. Díaz-Guillén<sup>b</sup>; U. Amador<sup>c</sup>; A. F. Fuentes<sup>a\*</sup>**

<sup>a</sup>Cinvestav Unidad Saltillo, Apartado Postal 663, 25000-Saltillo, Coahuila, Mexico.

<sup>b</sup>División de Estudios de Posgrado e Investigación, Instituto Tecnológico de Saltillo, 25280-Saltillo, Coahuila Mexico.

<sup>c</sup>Facultad de Farmacia, Departamento de Química y Bioquímica, Universidad San PabloCEU, Urbanización Montepríncipe, 28668 Boadilla del Monte, Madrid, Spain.

**ABSTRACT**

Lanthanide oxides with the  $\text{Ln}_2\text{B}_2\text{O}_7$  general stoichiometry ( $\text{B} = \text{Sn}, \text{Ti}, \text{Hf}, \text{Zr}$ ) have attracted considerable attention over the past few years because of their high thermochemical stability and structural flexibility susceptible to alteration via processing and/or doping. Moreover, the series exhibit many chemical and physical properties of scientific and technological relevance. Some members display significant oxygen ion conduction at high temperatures and/or low thermal conductivity; some others are highly tolerant to radiation damage and show great potential to incorporate actinides in solid solutions. Depending on the  $\text{R}_{\text{Ln}}/\text{R}_{\text{B}}$  size ratio,  $\text{Ln}_2\text{B}_2\text{O}_7$  oxides will adopt either the fully disordered anion deficient fluorite structure ( $\text{R}_{\text{Ln}}/\text{R}_{\text{B}} < 1.46$ ) or its ordered derivative, the pyrochlore structure ( $\text{R}_{\text{Ln}}/\text{R}_{\text{B}} \geq 1.46$ ); factors such as processing conditions or the nature of chemical bonding play also an important role in determining the specific degree of structural order/disorder of any particular composition. Therefore,  $\text{Ln}_2\text{B}_2\text{O}_7$  oxides are ideal systems to analyze structure/microstructure-properties relationships. In this work, we present the mechanochemical synthesis, structural characterization and electrical properties of the  $\text{Gd}_2\text{Hf}_{2-x}\text{Zr}_x\text{O}_7$  system ( $x = 0, 0.4, 0.8, 1.2, 1.6$  and  $2$ ). The evolution of the starting mixtures with milling time was followed by standard XRD and Raman spectroscopy; to analyze the evolution of defects and disorder with temperature, as-obtained powders were also fired at two different temperatures and characterized by different techniques including synchrotron XRD. Electrical properties were measured by using impedance spectroscopy as a function of temperature and frequency; conductivity and activation energies for oxide ion migration in the system were calculated as a function of the Hf/Zr ratio.

**Keywords:** Mechanical milling, Order-disorder transition, pyrochlore, Fluorite

\* Corresponding author:

Dr A. F. Fuentes, tel.: +52 844 4389617; email: fuentesaf@live.com

**Preparation of sulfonic-functionalized mesoporous carbon as ion-exchange material for fuel cells applications**

**D. Morales-Acosta<sup>a\*</sup>; R. Benavides<sup>a</sup>; L. Melo<sup>a</sup>; N. Sanchez-Padilla<sup>b</sup>,  
F.J. Rodríguez-Varela<sup>b</sup>**

<sup>a</sup>Centro de Investigación en Química Aplicada, Depto. Procesos de Transformación, Blvd. Enrique Reyna Hermosillo 140, Saltillo, Coahuila, 25294, México.

<sup>b</sup>Programa de Sustentabilidad de los Recursos Naturales y Energía, Cinvestav Unidad Saltillo, Av. Industria Metalúrgica 1062, Parque Industrial Ramos Arizpe. Ramos Arizpe, Coahuila, 25900, México.

**ABSTRACT**

In this study sulfonic-functionalized mesoporous carbon (sMC) was prepared for the development of Nafion/sMC composite membranes. The MC was synthesized via self-assembly in aqueous solution from Resorcinol and Formaldehyde as carbon precursors and through a carbonization process carried out at several pyrolysis temperatures. The sMC materials were sulfonated using concentrated sulfuric acid. The influence of carbonization temperature on the pore structure and acidity were evaluated. The sMC materials were characterized by Fourier-Transform Infrared Spectroscopy, Raman Spectroscopy, and an indirect titration method to demonstrate the successful modification of -SO<sub>3</sub>H groups on the carbon surface. N<sub>2</sub> adsorption-desorption and transmission electron microscopy were used to characterize the mesoporous structure and pore structure parameters. The results indicate that the mesoporous structure remain stable after the pyrolysis process but the content of -SO<sub>3</sub>H groups depend mainly on the pyrolysis and sulfonation temperatures, which are essential for developing Nafion/MCs composite membranes with high densities of -SO<sub>3</sub>H groups.

**Keywords:** Mesoporous carbon, Sulfonation, Sulfonic acid groups, Fuel cells

\* Corresponding author:

D. Morales Acosta, 52 +844 438-9830 (Ext. 1422), 25294, diana.morales@ciqa.edu.mx

**Synthesys of carbon nanomaterials doped with sulfur as  
electrocatalysts in fuel cells**

**E. Montiel-Macias<sup>a,\*</sup>; P. B. Balbuena<sup>b</sup>; A. M. Valenzuela-Muñiz<sup>a</sup>; Y. Verde-Gómez<sup>a</sup>**

<sup>a</sup>Instituto Tecnológico de Cancún, Av. Kabah Km. 3, Cancún, Q. Roo, México, 77515.

<sup>b</sup>Department of Chemical Engineering, Texas A&M University, TAMU 3122, College Station, TX, USA, 77843.

**ABSTRACT**

In recent years, many efforts have been made to develop new materials that could replace or reduce the use of Pt in fuel cells electrocatalysts. Under this consideration, different materials based on carbon doped with heteroatoms applied as catalysts or catalyst supports in fuel cells have been investigated, e.g. N, B, P and S. In this work sulfur-doped carbon nanomaterials were synthesized by a chemical vapor deposition modified method, where toluene and thiophene were used as sources of carbon and sulfur, respectively. Ferrocene was used as a growing precursor. Different synthesis scenarios were evaluated to determine the optimal synthesis conditions. Physical and chemical characterization was performed by X-Ray Diffraction, Scanning and Transmission Electron Microscopy, in order to determinate structural and morphological properties. The chemical elemental analysis was done by energy dispersive spectroscopy.

**Keywords:** Sulfur doped carbon, Electrocatalysts, Fuel Cells

\* Corresponding author:

Elizabeth Montiel Macias, phone +529988807432, elizabethmontielmacias@hotmail.com

**Photoelectrochemical behavior of  $\text{TiO}_2$  nanorods film decorated by silver nanoparticles**

**J. V. Medina-Flores<sup>a,\*</sup>; M. Corrales-Luna<sup>a</sup>; A. Romero-Hernandez;  
E. M. Arce-Estrada<sup>a,\*</sup>; A. Manzo-Robledo<sup>b</sup>**

<sup>a</sup>Instituto Politécnico Nacional. ESIQIE. Departamento de Ingeniería en Metalurgia y Materiales, México, D.F.

<sup>b</sup> Instituto Politécnico Nacional. ESIQIE. Laboratorio de Electroquímica y Corrosión, México, D.F.

**ABSTRACT**

The photoelectrochemical activity of  $\text{TiO}_2$ -based heterostructures was evaluated in alkaline medium for oxygen evolution reaction, OER. The heterostructures were employed as photoanodes and were fabricated by attaching silver nanoparticles to  $\text{TiO}_2$  nanorods, grown on FTO substrate, by means of an electrodeposition, the quantity of deposited Ag was controlled by the time of deposit and were performed at 5, 10, 15 and 20 seconds. Field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD) and electrochemical technics were used to characterize the synthesized heterostructures. SEM analysis showed the formation of vertically oriented nanorods about 100 nm in diameter, constituted by nanowires close to 10 nanometers in diameter. X-ray diffraction showed the formation of rutile  $\text{TiO}_2$  without the presence of another phase. The photoelectrocatalytic activity of the synthesized materials was evaluated in 0.1 M KOH using open circuit potential, cyclic voltammetry, chronoamperometry and electrochemical impedance spectroscopy (EIS) under ultraviolet 254 and 365 nm. The recorded data from the electrochemical evaluation demonstrated the presence of Ag increases photoelectrochemical activity obtaining a maximum photocurrent of  $33.34 \mu\text{A}/\text{cm}^2$  under UV irradiation at a wavelength of 254 nm for the material with 5 second of deposit and a photocurrent of  $91.75 \mu\text{A}/\text{cm}^2$  under UV 365 nm for 10 seconds of deposit material. According to the results, the presence of silver nanoparticles extends the light absorption to larger wavelength and this is really important because the visible region from solar spectrum is the largest proportion.

**Keywords:** Oxygen evolution reaction, Heterostructures, Nanorods, Nanoparticles

\* Corresponding author:

Dr Elsa M. Arce Estrada, (+55) 5729 6000 ext. 54212 fax 54267, earce@ipn.mx

**Effect of the graphene and other supports for the oxygen reduction and evolution in alkaline media**

**M. A. Garcia-Contreras<sup>a,b\*</sup>; P. Hosseini-Benhangi <sup>a</sup>; A. Taheri- Najafabadi <sup>a</sup>;  
E.Gyenge<sup>a</sup>**

<sup>a</sup> Dept of Chem and Biological Engng & Clean Energy Res Center, The University of British Columbia, 2360 East Mall, Vancouver, BC, Canada V6T 1Z3

<sup>b</sup>Dept of Chemistry, ININ, Carr. México-Toluca s/n, La Marquesa Ocoyoacac, Edo. De Méx 52750

**ABSTRACT**

Graphene holds promise for many key areas of research including energy storage and conversion, biotechnology, novel electronic devices and so forth. Bifunctional O<sub>2</sub>cathodes which can catalyze both ORR (O<sub>2</sub> reduction reaction) and OER (O<sub>2</sub> evolution reaction) are the backbone of rechargeable metal-air batteries as well as regenerative fuel cells. Mn oxides have been vastly employed as a robust cost-effective multifunctional and environmental friendly electrode material in battery industry. The electrolytic  $\gamma$ -MnO<sub>2</sub> is known as the most electrochemically active crystallographic form of MnO<sub>2</sub> for ORR in alkaline media. However, poor OER electrocatalytic activity in alkaline media impairs its application for bi-functional catalysts. This could be overcome by adding another class of catalyst active for OER to the MnO<sub>2</sub>. LaCoO<sub>3</sub>, also known as a perovskite-type oxide, has been reported to display electrocatalytic activity for OER in alkaline electrolytes in comparison to Pt or MnO<sub>x</sub> as well as durability. A literature search on other bifunctional electrodes shows that the MnO<sub>2</sub>-perovskite catalytic system is very competitive with other catalysts presented in the literature, while having the advantage of cost efficiency and easy preparation methodology. Our research aimed at investigating the effect of the support on the performance of MnO<sub>2</sub>-based catalysts for both ORR and OER with long cycle life. The mechanisms for OER and ORR of the mixed catalysts and the role of support were investigated by a combination of surface characterization methods and electrochemical techniques.

LaCoO<sub>3</sub> was synthesized via co-precipitation methods. A novel approach toward electrochemical exfoliation of graphite assisted by ionic liquids (ILs) was used to synthesize both graphene and N-doped graphene. The catalyst layer consisted of MnO<sub>2</sub>:LaCoO<sub>3</sub>:Support:Nafion with a weight ratio of 1:1:1:0.67. The support varied from the electrochemically synthesized graphene and N-doped graphene to graphitized C. Cyclic voltammetry tests were performed in O<sub>2</sub> and N<sub>2</sub> saturated 6 M KOH at 293 K to investigate the electrocatalytic activity of the MnO<sub>2</sub>-LaCoO<sub>3</sub> catalyst on different supports as well as its long-term durability. Raman and X-ray photoelectron spectroscopies as well as SEM analysis were employed to further characterize the catalyst layer.

**Keywords:** Manganese dioxide electrode, Bifunctional oxygen electrocatalyst, Oxygen reduction reaction

\*Corresponding author: Miguel García, Tel. 52553297200 Ext. 12281; miguel.garcia@inin.gob.mx





## **Bimetallic cores decorated with Pt as electrocatalyst for PEM fuel cell**

**E. Flores-Rojas<sup>a,\*</sup>; F. Godínez-Salomón<sup>a</sup>; O. Solorza-Feria<sup>a</sup>; J. F. Pérez-Robles<sup>b</sup>**

<sup>a</sup> CINVESTAV-IPN. Unidad Zacatenco, Av. Instituto Politecnico Nacional 2508, San Pedro Zacatenco, Gustavo A. Madero, 07360 Ciudad de México, Distrito Federal, México.

<sup>b</sup> CINVESTAV-IPN. Unidad Querétaro, Libramiento Norponiente 2000, Fraccionamiento Real de Juriquilla, 76230, Querétaro, México.

### **ABSTRACT**

Electrocatalysis is a broad field of research with many different electrochemical reactions and catalyst materials. Significant work has been done over the last decades to understand the effect of particle size on electrocatalytic reactions in order to improve the sluggish kinetics of the cathodic Oxygen Reduction Reaction, looking for increasing efficiency, stability and durability for a long time of the electrocatalyst. New and more stable materials are employed diminishing the content of noble metals (e.g. Pt or Pd) in electrocatalysts and these represent the most challenging ambitions on the PEM fuel cells performance.

The possibility of manipulating structures and designing new arrangements in core-shell electrocatalysts combining processes and new synthesis techniques was the major motivation to carry out this research work. In order to continue with those goals, bimetallic solid solutions decorated with Pt catalysts were prepared and characterized to investigate their activity for the molecular oxygen reduction reaction. Solid solutions materials with different compositions used as core were synthesized by the High Energy Milling technique and physically supported on carbon by sonication. Solid solutions decorated with Pt were prepared by the Galvanic Displacement process to form electrocatalysts ( $\text{Co}_{70}\text{-Ni}_{30}\text{@Pt/C}$ ,  $\text{Co}_{50}\text{-Ni}_{50}\text{@Pt/C}$  and  $\text{Co}_{30}\text{-Ni}_{70}\text{@Pt/C}$ ) and studied in acid medium. X-Ray Diffraction was used for phases' identification and structural characterization of the cores while their bulk compositions were analyzed by Scanning Electron Microscopy with X-Ray microanalysis (SEM/EDS). Transmission Electron Microscopy was used to determine particle size in the final electrocatalysts. Electrocatalytic activity was evaluated by Cyclic Voltammetry (CV) and Rotating Disk Electrode (RDE) and the results conducted to a homogenous distribution particles with 15 nm average particle in size. Around 80 mA/mg<sub>Pt</sub> and 0.4 mA/cm<sup>2</sup><sub>Pt</sub> of Mass Activity and Specific Activity respectively at 0.9 V for the three catalysts.

**Keywords:** Solid solution, High energy milling, Galvanic displacement reaction

\* Corresponding author:

Ernesto Flores-Rojas, +52 (55) 57473800 ext 4473, México D.F., 07360, México, efloresr@cinvestav.mx

**Role offunctionalized carbon support on the electroactivity of  
Platinum and Palladium**

**A. Godinez-Garcia<sup>a</sup>;Dominic F. Gervasio<sup>b</sup>**

<sup>a</sup>Departamento de Ingenieria de Procesos e Hidraulica, Universidad Autonoma Metropolitana, Unidad Iztapalapa, Av. San Rafael Atlixco 186, 09340 Mexico City, Mexico.

<sup>b</sup>The University of Arizona, Department of Chemical and Environmental Engineering. Harshbarger 108, 1133 E. James Rogers Way, Tucson, Az 85721-0011, USA.

**ABSTRACT**

Platinum and Palladium nanoparticles were supported on carbon nanotubes and nanofibers using high-intensity sonication in order to study the support effect on the electroactivity of the palladium and platinum nanoparticles for the oxygen reduction reaction (ORR). Scanning electronic microscopy and electrochemical techniques were used for analyzing microstructure and morphology of the synthesized electrocatalysts. The results showed that acid functionalization of the used supports increased the electrochemical double layer, that it is a consequence of an increasing of the surface area. However, the electroactivity decreased because these functionalized supports also decrease the electrical conductance as the electrochemical characterization showed.

**Keywords:** Platinum and Palladium, Nanomaterials, Carbon nanotubes, Carbon nanofibers, Electrocatalysts

\* Corresponding author:

A. Godínez García, +52-55-58044600, ext. 1244, 09340, Mexico DF, Mexico, andgodinez@xanum.uam.mx

**Response of cerium incorporation at TiO<sub>2</sub> nano-structures for induced electrochemical and capacitive processes at neutral conditions**

**A. A. Flores-Caballero<sup>a</sup>; J. R. Gómez-Romero<sup>b</sup>; C. García-Mendoza<sup>b</sup>;  
L. Lartundo-Rojas<sup>c</sup>; A. Manzo-Robledo<sup>a,\*</sup>**

<sup>a</sup>Laboratorio de electroquímica y corrosión. Departamento de Ingeniería Química. Escuela Superior de Ingeniería Química e Industrias Extractivas (ESIQIE)-IPN, Distrito Federal, México, 07300.

<sup>b</sup>Laboratorio de Ecocatálisis. Universidad Autónoma Metropolitana, Unidad Iztapalapa, Distrito Federal, México, 09340.

<sup>c</sup>Centro de nano ciencias y Micro y Nanotecnologías (CNMN)-IPN, Distrito Federal, México, 07738.

**ABSTRACT**

Cerium-doped TiO<sub>2</sub> (1 and 3 %wt. Ce) has been synthesized by the sol-gel route using titanium butoxide and cerium (III) nitrate hexahydrate as precursors. The samples obtained were calcined at 400°C. Techniques such as X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), UV-Vis diffuse reflectance, BET surface area, infrared spectroscopy (FTIR), cyclic voltammetry (CV), lineal sweep voltammetry (LV) and electrochemical impedance spectroscopy (EIS), were employed to characterize the synthesized materials towards induced electrochemical reactions linked with oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) zones. According to XPS analysis, some shifts in the binding energies were observed due to addition of cerium, as well as textural and vibrational changes into the structure. Also, it was found that less capacitive processes are induced due to cerium incorporation, as demonstrated by CV and EIS. The flat band potential and the band gap calculated were in the order Ce<sub>3.0</sub>TiO<sub>2</sub> < Ce<sub>1.0</sub>TiO<sub>2</sub> < TiO<sub>2</sub> < P25, indicating that the charge-transfer processes promoted at the electrode-electrolyte interface are more efficient at titanium dioxide doped with 3 % wt. Ce. These properties are highly related with particle size-distribution given by TiO<sub>2</sub>-cerium-structure alteration, according to XRD and TEM analyses.

**Keywords:** Semiconductors, Doped titanium dioxide, Sol- gel synthesis, Photo-electrochemistry, Interfacial processes

\* Corresponding author:

A. Manzo-Robledo, 52-1-(55) 57-29-60-00 Ext. 54246, amanzor@ipn.mx

**Nanostructured ionic conductors thin films for solid oxide fuel cells  
deposited by ultrasonic spray pyrolysis**

**M. F. García Sánchez<sup>a,\*</sup>; I. Ponce Rosas<sup>b</sup>; A. Benítez<sup>b</sup>; B. M. Monroy Pelaez<sup>b</sup>;  
J. Santoyo<sup>c</sup>; G. Santana<sup>b</sup>**

a Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas. Instituto Politécnico Nacional, Av. I.P.N. 2580, Gustavo A. Madero, 07340, México .D.F

b Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México. A.P. 70-360, Coyoacán, C.P. 04510, México, D.F

c Departamento de Física, CINVESTAV-IPN, A.P. 14-740, C.P. 07000, México, D.F

**ABSTRACT**

Nanostructured thin films of yttrium and ytterbium stabilized zirconia, and ceria have been prepared on crystalline silicon substrates by ultrasonic spray pyrolysis using acetylacetonates of zirconium, yttrium, ytterbium and cerium as metallo- organic precursors. The morphology, structure and electrical properties were studied by X ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), ellipsometry, atomic force microscopy (AFM) and impedance spectroscopy (IS). The substrate temperature was optimized for obtaining smooth, dense and homogeneous nanocrystalline films with grains sizes as low as 10 nm. The influence of thermal annealing at 650 °C on the films was analyzed. The activation energy measured for the grains was similar to that reported in bulk for these materials, but this parameter was reduced in the grain boundaries, increasing the total conductivity of material. It is related to small size of grains and the close boundaries obtained with the optimized conditions. The films obtained are good candidates for electrolytes in solid oxide fuel cells (SOFC) operating at lower temperatures.

**Keywords:** Stabilized zirconia, Nanostructure, Ultrasonic spray deposition

**Synthesis of carbon nanotubes doped with nitrogen towards the electroreduction of oxygen in alkaline media**

**I. Zeferino González\*; G. Rosado Ortíz; A.M. Valenzuela Muñiz; J.Y. Verde Gómez**

Instituto Tecnológico de Cancún, Av. Kabah Km. 3, Cancún, Q.R., México, 77500.

**ABSTRACT**

The unique properties of carbon nanotubes, makes them ideal materials for many applications, however, for specific applications it is necessary to modify the properties of materials. Doping of carbon nanostructure is one of the most effective ways to change their properties. Incorporating nitrogen atoms into the carbon structure can drastically change their properties. One of the most outstanding potential applications found for carbon doped is as a catalyst for oxygen reduction reaction (ORR) in fuel cells. So, in this work nitrogen doped carbon nanotubes (N-CNTs) was synthesized simultaneously by the chemical vapor deposition modified method. Pyridine was used as carbon and nitrogen precursor and ferrocene as catalyst for the nanotubes growth. The composite material was investigated using scanning electron microscopy, transmission electron microscopy, X ray diffraction and X-ray photoelectron spectroscopy. The electrocatalytic performance of the material was evaluated towards the oxygen reduction reaction by linear sweep voltammetry measurements. A catalyst-coated rotating disk electrode at different rotation rates in 0.1 M KOH solution was evaluated. The electrocatalyst N-CNTs improved the electrocatalytic activity for ORR which proceeds in a nearly four-electron pathway. The favorable result was due to the higher content of nitrogen that was incorporated into the structure of carbon. Moreover, according the characterization studies indicated that pyrrolic nitrogen may act as active sites of catalysts for ORR.

**Keywords:** Nitrogen doped carbon nanotubes, Chemical vapor deposition, Oxygen reduction reaction

\* Corresponding author:

Isaias Zeferino González, T: 52 (998) 8807432 ext: 1020, 1012, E: zeferino.isaias@yahoo.com.mx

**Electrochemical evaluation of the Pd-Fe<sub>3</sub>O<sub>4</sub>/C nanocatalyst as highly active anode for the oxidation of organic molecules**

**J.E. Solis-Tobías<sup>a</sup>; J.A. Díaz-Guillén<sup>a</sup>; P. Meléndez-González<sup>b</sup>; F.J. Rodríguez-Varela<sup>b</sup>**

<sup>a</sup>Instituto Tecnológico de Saltillo, 25280-Saltillo, Coahuila Mexico

<sup>b</sup>Programa de Sustentabilidad de los Recursos Naturales, Cinvestav Unidad Saltillo, Av. Industrial Metalúrgica No. 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, Coah., México, 25900.

**ABSTRACT**

The novel 20 % Pd-Fe<sub>3</sub>O<sub>4</sub>/C nanostructured material (Pd:Fe<sub>3</sub>O<sub>4</sub> atomic ratio of 1:1) was synthesized using NaBH<sub>4</sub> as reducing agent. The catalysts was evaluated as anode for the ethanol, ethylene glycol and glycerol oxidation reactions (EOR, EGOR and GOR, respectively) and compared with a 20 % Pd/C material in alkaline media. The results showed that Pd-Fe<sub>3</sub>O<sub>4</sub>/C is highly active for the oxidation of the five organic molecules. In all cases, it exhibited similar or even lower on-set potentials compared to Pd/C. Moreover, it showed higher peak current densities for the EOR, EGOR and GOR related to the monometallic anode. As an example, the on-set potential and oxidation peak current density of the EGOR (0.5 M) were – 300 mV (vs. SHE) and 83.21 mA/cm<sup>2</sup> at Pd-Fe<sub>3</sub>O<sub>4</sub>/C, compared to – 300 mV (vs. SHE) and 69.18 mA/cm<sup>2</sup> at Pd/C. Similar enhancement in catalytic activity was observed for the two other reactions. The results suggested that Pd-Fe<sub>3</sub>O<sub>4</sub>/C is a suitable anode for Direct Alcohol Fuel Cells, not only for its high catalytic activity, but also because it contains a cheap co-catalyst such as magnetite.

**Keywords:** Pd-Fe<sub>3</sub>O<sub>4</sub>/C nanostructured catalysts, Oxidation of organic molecules, Alkaline media, Direct alcohol fuel cells

\* Corresponding author:

F.J. Rodríguez-Varela, Phone number: T: 52(844)438-9600 Ext. 8526, E: javier.varela@cinvestav.edu.mx

## **Environmental aspects**



**Solar radiation measurements to optimize a PV system according to local weather conditions**

**V. Juárez Casildo<sup>a</sup>; M. Tufiño Velázquez<sup>b</sup>; A. Yunez Cano<sup>c</sup>;  
R. de G. González Huerta<sup>a\*</sup>**

<sup>a</sup>ESIQIE-IPN, Lab. Electroquímica y Corrosión, UPALM, CP 07738, México, D.F.

<sup>b</sup>ESFM-IPN, Laboratorio de Física Avanzada, UPALM, CP 07738, México, D.F.

<sup>c</sup>CIITEC-IPN, Cda. Cecati s/n, Col. Sta. Catarina, CP 02250 Azc., México D.F.

**ABSTRACT**

The accelerated growth of population has brought an increase in the energy demand for the production of goods and services. This fact has involved at the same time high cost environmental damages as well as economic troubles such as global warming and increase in the electricity costs. In Mexico, greenhouse gas emissions are mainly due to the transport sector and electricity production. Regarding the last sector, electrical power consumption per household is around 33% of total energy production. Installing a photovoltaic (PV) system provides several benefits to a homeowner; as he is producing his own electricity, his utility bills will be lower.

PV has become one of the most promising technologies because its energy source is free and environmental friendly. However, we should consider the weather conditions, including daily and seasonal changes of solar irradiance. The interest in the use of solar energy has promoted the measure and recording of local weather in potential sites to combine its use with sustainable power sources. In this work, solar radiation measurements from a meteorological monitoring station placed in the roof of a sustainable house located in the north side of Mexico City was analyzed. It was determined an average annual irradiation of 4,217 W/m<sup>2</sup>-day less than 5025 W/m<sup>2</sup>-day, which was reported by CONUEE. In order to meet the continuous power delivery from a PV system, it is often used by the use of high capacity and environmental non-friendly storage batteries. One option to solve this problem is to use hydrogen as a storage system and carrying medium of energy from renewable sources, in order to increase the reliability of a proposed stand-alone system. From this analysis the average monthly irradiance incident on the photovoltaic system to determine an appropriate charge and achieve optimization was obtained.

The authors thank CONACYT: Programa de Redes Temáticas (RTH2) Projects 252003; and IPN-SIP multidisciplinary projects 1683 and 1725.

**Keywords:** Solar radiation, PV system, Local weather, Hydrogen storage system

\* Corresponding author:

Rosa de Guadalupe González Huerta, (+52) 55 57296000 ext 54246, rosgonzalez\_h@yahoo.com.mx

**Cellulose, hemicellulose and lignin from urban waste to saccharides by hydrolysis for biohydrogen production**

**J. C.Gómora-Hernández<sup>a,b</sup>; M. C. Hernández-Berriel<sup>b</sup>; S. M. Fernández-Valverde<sup>a,\*</sup>**

<sup>a</sup>Depto. de Química, Instituto Nacional de Investigaciones Nucleares, A.P. 18-1027, Mexico D.F. C.P.11801, Mexico. Tel. 5553297200 ext 12277

<sup>b</sup>Instituto Tecnológico de Toluca, Avenida Tecnológico s/n, Fraccionamiento la Virgen, Metepec, Estado de México, México. C.P. 52149. Tel. 7222087200

**ABSTRACT**

In Mexico the organic fraction of municipal solid waste (>50%) is disposed of in landfills or open dumps. Upon degradation they contribute to pollution affected by the emission of CH<sub>4</sub> and CO<sub>2</sub>, H<sub>2</sub>S also is formed and the fatty acids produced are leachate producing soil erosion. The fruit and vegetable fraction presented in urban waste is important for saccharides content that could be used for biohydrogen production. However the polysaccharides such as: cellulose, hemicellulose and lignin are not degraded by hydrogen produced mesophilic bacteria. An effective treatment for polysaccharides is hydrolysis in acid media in order to transform the carbohydrates in saccharides. The hydrolysis in acid media is an effective method to do that in an economic and rapid way. Between the acids to made the hydrolysis, phosphoric acid is one of the choice acids: after neutralization can apports phosphate salts that could be used by the bacterias as nutrients and also play a role like media buffer solution. During hydrolysis at temperatures of 80 °C or higher aromatic compounds could produce inhibiting the bacteria growing. In this research the fruit and vegetable fraction equivalent to that studied before for biohydrogen production was investigated for hydrolysis in concentrated phosphoric acid. In vials of 50 mL one gram of dried waste was mixed with 10 mL of phosphoric acid (83 %), the vials were sealed and heated at 50 °C in a thermostated shaking bath. A sample was taken every hour, filtered, the solid was washed twice with water and once with ethanol and dried at 50 °C until constant weight and then analyzed by Infrared Spectroscopy (IR). In the blank sample the characteristics vibrations of cellulose, hemicellulose and lignin were found, they disappear with reaction time. The  $\alpha$ -glucosidic bond (952 cm<sup>-1</sup>) related to saccharose and starch, vanish after 10 h reaction time also lignin (1590-1510 cm<sup>-1</sup>) disappears before this reaction time. The  $\beta$ -glucosidic bond (889 cm<sup>-1</sup>) related to cellulose and hemicellulose decreases but is still present after 25 h reaction time. The saccharides were recovered by evaporation, the yield in dried base was 0.61 g/g dry waste and 68.2% related to total volatile solids.

**Keywords:** Biohydrogen production, Organic waste, Hydrolysis, Polysaccharides degradation

\*Suilma M. Fernández-Valverde, +52 01 55 53 29 72 00 ext. 12277: suilma.fernandez@inin.gob.mx



## **Hydrogen production research in Mexico: A Review**

**V. Collins-Martínez; M. J. Meléndez Zaragoza; A. López Ortiz\***

Departamento de Ingeniería y Química de Materiales, Centro de Investigación en Materiales Avanzados, S.C., Miguel de Cervantes 120, Chihuahua, Chih., México, 31136, México.

\*Tel: +052 6144394815, mail: alejandro.lopez@cimav.edu.mx

### **ABSTRACT**

The insertion of the hydrogen technologies into Mexico's energy portfolio is a complex matter. Historically, the energy sector has been monopolized by the government. However, very recently (August 2014) an energy reform bill approved by the Mexican Congress and ratified as a law by the president allowed foreign investment in the energy sector. In this context, there is a great opportunity for alternative energy and specifically for hydrogen technologies to flourish within Mexico. Specifically, the opportunity for the hydrogen production research activities to contribute to the advance and possible application of the related hydrogen technologies is today of paramount importance. The present paper is aimed to present a review of the hydrogen production research activities in Mexico. Main research activities reflected in Journal publications and conference proceedings within the last seven years resulted in the following topics and contributions: Hydrogen production (HP) from biological processes and wastes 40.4%, followed by HP through conventional and non-conventional fuels (CO<sub>2</sub> capture & Catalysis) 22.4%, HP by photocatalysis & photo-electrocatalysis 14.1%, HP systems and controls 12.2%, theoretical and thermodynamic studies for HP 7.7%, and HP by electrolysis 3.2%. A wide variety of potential applications can be followed by these contributions, while the spread of this research can be a key for future national or international collaborations that may strengthen this important area within the energy sector to take advantage of the upcoming opportunities in the country.

**Keywords:** Hydrogen production research, Mexico

\* Corresponding author:

Alejandro Lopez Ortiz, Tel: +052 614 4394815, email: alejandro.lopez@cimav.edu.mx

**XV International Congress of the Mexican Hydrogen Society**  
**September 22 – 25, 2015**  
**Mexico, D.F.**

**Using hydrogen fuel and bio-ethanol in internal combustion engines to  
reduce emissions of greenhouse gases**

**J. D. Becerra-Ruiz<sup>a</sup>; R. G. Gonzalez-Huerta<sup>b</sup>; G. Macias-Bobadilla<sup>c\*</sup>**

<sup>a</sup>. División de Estudios de Posgrado, Facultad de Química, Universidad Autónoma de Querétaro. Cerro de las Campanas S/N col. Las Campanas. C.P. 76010, Querétaro, Qro. Mexico.

<sup>b</sup>. ESIQIE-IPN, Laboratorio de Electroquímica y Corrosión, C.P. 07738, D.F. México.

<sup>c</sup>. División de Estudios de Posgrado, Facultad de Ingeniería, Universidad Autónoma de Querétaro. Cerro de las Campanas S/N col. Las Campanas. C.P. 76010, Querétaro, Qro. Mexico.

**ABSTRACT**

This work investigated the effect of hydrogen-oxygen blends and bioethanol addition on the performance of a gasoline engine. Hydrogen-oxygen blend was added in the air intake system and bioethanol was mixed with gasoline into the vehicle tank. The tests were performed in both cases independent and additive combination, in a gasoline engine 2.0 L corresponding to a vehicle NISSAN - Sentra 2007, which were made modifications for adding these mixtures, were measured the operating temperature of the engine and exhaust fumes. The standard hydrogen-oxygen enrichment contributed to the decreased HC, CO<sub>2</sub> and CO emissions. In addition to this was found in experiments that can be further improved combustion if bioethanol is added, as indicated by some previously published studies, where the mixture of gasoline - bioethanol should not exceed 85-15% ratio respectively for engines they are not Flex-Fuel. Discussions were focused on the results obtained with the different proportions of bioethanol mixed with gasoline and hydrogen-oxygen blend, as well as measurements of the parameters of engine temperature, oxygen expelled by the engine and were compared with those measured by the equipment automotive emissions analysis BEA gases v3.70-EURO-W (AMM-000-B6) series of Bosch. Because all, this is left to discussion that using blends of gasoline with bioethanol and hydrogen-oxygen enriched air reduces emissions of greenhouse gases from the engine and increases the performance of fossil fuel. One of the most important advantages of the systems is that current technology is used and only minor adjustments need to be done to integrate a hybrid system.

**Keywords:** Gasoline engines, Hydrogen enriched air, Enriched gasoline Bioethanol

\*Corresponding author:

Gonzalo Macías-Bobadilla, Universidad Autónoma de Querétaro, Querétaro, México,  
T: 442 252 2912, E: g.macias@uaq.mx



## Miscellaneous

**Protic ionic liquids as “all-in-one” solvent toward the  
green synthesis of metal oxides**

**L. Álvarez-Contreras<sup>a</sup>; J. Ledesma-García<sup>b</sup>; L. G. Arriaga<sup>c</sup>; M. Guerra-Balcázar<sup>b</sup>;  
N. Arjona<sup>d,\*</sup>**

<sup>a</sup>Centro de Investigación en Materiales Avanzados S. C., Chihuahua, Chih., C.P. 31109, México.

<sup>b</sup>Facultad de Ingeniería, División de Investigación y Posgrado, Universidad Autónoma de Querétaro, Querétaro, Qro., C.P. 76010, México.

<sup>c</sup>Centro de Investigación y Desarrollo Tecnológico en Electroquímica S. C., Pedro Escobedo, Qro., C.P. 76703, México.

<sup>d</sup>Centro de Investigación y Desarrollo Tecnológico en Electroquímica S. C., Unidad Tijuana, Tijuana, B. C., C.P. 22444, México.

**ABSTRACT**

Ionic liquids have unique chemical properties which make them ideals for applications in chemical and electrochemical processes. The 2-hydroxy ethylammonium formate protic ionic liquid was synthesized by a Brønsted acid-base reaction and used as “all-in-one” solvent, it was selected because of the nature of their ions. In this work, Cu, Ni and Fe-based salts were used toward the syntheses of small metal oxide particles at room temperature and at low reaction times (less than 30 minutes). These materials were physicochemically characterized by TGA, TEM, XRD and XRF. According with those results, particles with sizes in the order of 1.5 to 10 nm were obtained. Furthermore, the use of those salts resulted in CuO, NiO and Fe<sub>2</sub>O<sub>3</sub> nanoparticles. In summary, this protic ionic liquid allowed to obtain small nanoparticles obeying most of the green chemistry principles.

**Keywords:** Electrocatalysis, Ionic liquids, Green chemistry

\* Corresponding author:

Noé Arjona, +52 (664) 660 20 54 ext. 4416. noe.arjona@yahoo.com.mx & wvelazquez@cideteq.mx

**Revising the molecular dynamics of hydrogen within the sulfur-ammonia  
photothermochemical cycle through NMR spectroscopy**

**R. Orozco-Mena<sup>a</sup>; R. Marquez-Montes<sup>a</sup>; J. Mendoza-Chacón<sup>a</sup>; E. Herrera-Peraza<sup>b</sup>; H.  
Romero-Paredes<sup>c</sup>; D. Chavez-Flores<sup>a</sup>; V. H. Ramos-Sánchez<sup>a,\*</sup>**

<sup>a</sup>Facultad de Ciencias Químicas, Universidad Autónoma de Chihuahua, Nuevo Campus Universitario,  
Circuito Universitario, Chihuahua, Chih., México. C.P. 31125.

<sup>b</sup>Centro de Investigación en Materiales Avanzados, S.C., Miguel de Cervantes #120, Complejo Industrial  
Chihuahua, Chihuahua, Chih., México. C.P. 31109.

<sup>c</sup>Universidad Autónoma Metropolitana Iztapalapa, San Rafael Atlixco #186, Iztapalapa, México D.F.,  
Mexico. C.P. 09340

**ABSTRACT**

Among thermochemical cycles, the sulfur family cycles have been shortlisted as the most promising routes to obtain hydrogen at large scale. A new photothermochemical cycle within the same family has been developed in recent years: the sulfur-ammonia (S-NH<sub>3</sub>) cycle. One of the major benefits of the S-NH<sub>3</sub> cycle is the production of H<sub>2</sub> at room temperature exploiting UV radiation by oxidation of aqueous (NH<sub>4</sub>)SO<sub>3</sub>.

We have already studied the photolytic oxidation of (NH<sub>4</sub>)SO<sub>3</sub>·H<sub>2</sub>O to produce H<sub>2</sub> under controlled and concentrated UV radiation using Raman microscopy to better understand the reaction dynamics and ultimately replicate such reaction within a solar reactor. It has been clearly revealed that water is required to promote photolytic oxidation of (NH<sub>4</sub>)SO<sub>3</sub>. Thus, at first sight, it seems rational to think that H<sub>2</sub> produced comes from water through direct splitting. However, the role of NH<sub>4</sub><sup>+</sup> ion in such reaction has been somehow neglected. Moreover the participation of the protons within NH<sub>4</sub><sup>+</sup> ion is yet unknown, in spite of the fact that they might be involved in the reaction mechanism that ultimately leads to hydrogen production.

Hence, this study aims to elucidate the reaction mechanisms involved in the oxidation of ammonium sulfite through an integral theoretical-experimental approach, consisting of isotopic substitution experiments carried out using NMR spectroscopy, which preliminarily have revealed the occurrence of two distinct proton entities in aqueous (NH<sub>4</sub>)SO<sub>3</sub> and (NH<sub>4</sub>)SO<sub>4</sub>.

**Keywords:** Solar hydrogen, Photothermochemical cycles, NMR, Sulfur-ammonia

\* Corresponding author: vramos@uach.mx, v.h.ramos.sanchez@gmail.com

