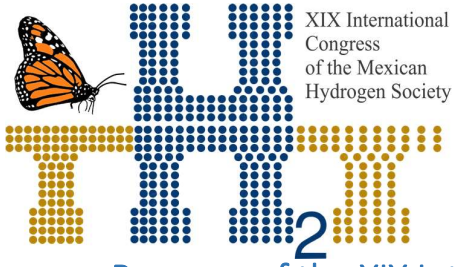

Program of the XIX International Congress of the Mexican Hydrogen Society

Time	Tuesday 01.10.2019			Wednesday 02.10.2019			Thursday 03.10.2019			Friday 04.10.2019		
08:00-08:30	Morelia City Center to UNAM transport											
08:30-09:00	Registration											
09:00-09:20	Pre-Congress course 1, part 1	Pre-Congress course 2, part 1.	Pre-Congress course 3, part 1	Opening (09:00-09:30)			005	011	031	009	017	085
09:20-09:40				Prof. Dr. Arturo Fernandez Madrigal Semblance (09:30-10:00)			008	034	045	023	048	083
09:40-10:00							021	035	071	024	074	077
10:00-10:20				Plenary Conference 1			067	038	096	Plenary Conference 3		
10:20-10:40							076	041	100			
10:40-11:00							084	050	113			
11:00-11:20	Coffee break											
11:20-11:40	Pre-Congress course 1, part 2	Pre-Congress course 2, part 2	Pre-Congress course 3, part 1	002	004	052	Plenary Conference 2			029	106	007
11:40-12:00				033	047	054				062	102	040
12:00-12:20				037	095	058				065	099	042
12:20-12:40				088	107	059	010		080	066	098	043
12:40-13:00				079	001	063	089	108	105	076	091	053
13:00-13:20				Sponsor exhibition						Clossening		
13:20-15:00	Lunch											
15:20-15:40				020	006	111	Posters session			UNAM to Morelia City Center transport		
15:40-16:00				022	036	082						
16:00-16:20				051	109	086						
16:20-16:40				055	101	087	HMS Assembly					
16:40-17:00				103	092	070						
17:00-17:30	UNAM to Morelia City Center transport											
18:00-19:00	Welcome cocktail			Cultural activity			Gala Diner					

Plenary conferences

Plenary Conference 1. Hydrogen production through photoelectrolysis: challenges and advances

Dr. Arturo Fernandez Madrigal
IER-UNAM

The International Energy Agency (IEA) proposed an urgent change in the energy sector, due to reduce the generation of greenhouse gases (GHG) and to a lesser extent due to the increase in prices and the decline in oil reserves, emphasizing the expression adopted in 1970, by the General Motors company, "Hydrogen Economy" used to define a new economic model based on hydrogen as a source of energy.

Hydrogen is called an energy vector, that is, it has to be extracted from other raw materials, for this a portion of energy has to be invested, currently more than 90% of the hydrogen produced is through fossil fuels; However, taking into account the proposal for a new energy model based on hydrogen as a fuel, it is vitally important to consider the advantages of renewable sources in favor of the clean production of the vector in question.

There are three different classes that supply the primary energy for hydrogen production: nuclear, fossil fuels and renewable energy. Within renewable energies the sun is the most important; It encompasses three forms of production, biological procedures, thermal decomposition and water electrolysis. This last process is considered the most environmentally friendly, basically consists of breaking down the water molecule into its constituent elements (hydrogen and oxygen). This research focuses on the concept of photoelectrolysis, which is based on this process. The concept of photoelectrolysis was proposed in 1972 by Fujishima and Honda and they demonstrated that a semiconductor with the appropriate properties submerged in an aqueous electrolyte, being illuminated with sunlight can transform the photon's energy into electrochemical energy which It can directly decompose the water molecule. The device where this process is carried out is called a photoelectrochemical cell (PEC).

The PEC is linked to various areas of science: the optical functions required to absorb as much solar radiation as possible and on the other hand the catalytic functions necessary for water separation, resulting in the conversion of solar energy into an energy product. useful hydrogen.

This presentation will address the various configurations developed for the construction of the PECs, as well as the various types of materials used, addressing the current art of these devices.

Plenary Conference 2. Balancing gravimetric and volumetric hydrogen density in MOFs: Computational discovery and experimental demonstration

Dr. Donald Siegel
Mechanical Engineering Department, University of Michigan

Metal organic frameworks (MOFs) are promising materials for the storage of hydrogen fuel due to their high surface areas, tunable properties, and reversible gas adsorption. Although several MOFs are known to exhibit high hydrogen densities on a gravimetric basis, realizing high volumetric capacities remains a challenge. Here, MOFs that achieve high gravimetric and volumetric H2 densities simultaneously are identified computationally, and demonstrated experimentally. More specifically, the hydrogen capacities of ~100,000 MOFs drawn from databases of known and hypothetical compounds were predicted using empirical correlations and direct atomistic simulations. Based on these predictions, promising MOF candidates were synthesized and evaluated with respect to their usable H2 capacities. Several MOFs predicted to exhibit high capacities displayed low surface areas upon activation, highlighting the need to understand the factors that control stability. Consistent with the computational predictions, several MOFs were experimentally demonstrated to exhibit an uncommon combination of high usable volumetric and gravimetric capacities. Importantly, the measured capacities exceed those of the benchmark compound MOF-5, the record-holder for combined volumetric/gravimetric performance. These materials-level capacities were subsequently used as input to project system-level performance. Finally, several machine learning algorithms were trained on this computationally-generated database. The relative accuracy of these algorithms was compared, with the most promising algorithm applied to predict H_2 capacities in an additional 400,000 MOFs. Our study illustrates the value of computational screening in pinpointing materials that optimize overall storage performance.

Plenary Conference 3. Biohydrogen production: A strategy for wastewater management

Dr. René Cardeña Dávila
Instituto de Ingeniería, Unidad Académica Juriquilla

In Mexico, wastewater is a problem due to low treatment coverage. Biological processes are the most important and necessary stage for water treatment, they have such a wide versatility that value-added products can be obtained from it. The biohydrogen is produced by biological means by the action of microorganisms by degrading the organic matter present in the water. A substrate with high carbohydrate content will provide better hydrogen productions, for example, agro-industrial or food industry wastewater. Among the most important biological processes of hydrogen production are dark fermentation, photo-fermentation, and bioelectrochemical processes. During dark fermentation, complex molecules are transformed into simple monomers that are easier to assimilate by microorganisms for hydrogen production. However, the dark fermentation only removes between 30 and 40% of the substrate initial, the organic matter that remains in the liquid phase is transformed into more oxidized compounds, mainly volatile fatty acids. These volatile fatty acids serve as a raw material in the photofermentation process or microbial electrolysis cells, obtaining better overall hydrogen yields and better treatment for wastewater.

Pre-congress courses

Pre-congress course 1: X-ray Photoelectron Spectroscopy (XPS): Fundamentals and applications.

Fis. Lazaro Huerta Arcos
Institute of Materials Research, UNAM.
lazaro@iim.unam.mx

XPS consists in measuring the kinetic energy of ionized electrons from the internal orbits of atoms. It is used to obtain quantitative information on chemical states and study the valence band of the first atomic layers of solid materials (1-100 Å) with high precision.

In this workshop, some theoretical and experimental aspects of the techniques will be discussed: X-ray Photoelectron Spectroscopy (XPS / ESCA), angular resolution (ARXPS), Ultraviolet Ray (UPS), Ionic Erosion Depth Profiles using XPS.

Strategies are presented to obtain more information on the technique and the appropriate parameters for measurements and adjustments in spectral deconvolution are detailed.

The main application in research is an analysis of oxidation states in various disciplines and fields such as thin films, nanomaterials, carbon, metals, polymers and surface functionalization, organic materials, tribology, diffusion processes, catalysis, semiconductor, and superconducting materials, among others.

Pre-Congress course 2. Scientific research publication from basic to applied science: papers and patents.

Dr. Ismeli Alfonso Lopez
Morelia Unit Institute of Materials Research, UNAM.

Scientific research has been generally classified in basic and applied, being in both cases necessary the publication of the obtained results. Similitudes and differences exist between their more important kinds of divulgation, being these papers and patents, respectively. For the case of papers no regulations exist about where publish, and generally English is the preferred language; meanwhile for the case of patents in each country exists only one submitting place, and it is mandatary its publication in the official language of that country. It is important to remark that the 80 % of the whole scientific-technical information on the world is published in patents, being then indispensable not only the search in papers data bases, but also of patents. In this course we will address the issue of similarities and differences between papers and patens, including writing and submitting techniques; and tools for scientific-technical information search. Exercises about writing of papers and patents will be also performed, including recommendations for a better presentation of figures.

Pre-Congress course 3. Powder X-ray diffraction, from the begging to the software.

Dra. Karina Suarez

Morelia Unit Institute of Materials Research, UNAM.

X-ray diffraction is a powefull tool for the characterization of new materials. In this quick course, the fundamentals of X-ray diffraction are revisited. Main concepts such as the crystal size, crystallographic data, miscrostrains, etc. are revised. Then, a small experimental session to improve the sample preparation and data collection is performed. The most common erros and a way to avoining they are presented. Finally, the most important software and crystallographic databases for data processing are presented. The Rietveld method is also revisited.