INSIGHT SEMINAR: Searching of photocatalysts for a clean future - hydrogen generation and CO2 reduction

LOURDES F. VEGA

April 11, 2024
12:00 to 13:00
Seminar Room

BIO:

Prof. Lourdes F. Vega is a Full Professor in Chemical Engineering, Acting Senior Director of the Petroleum Institute, devoted to Sustainable Fuels, from a broad perspective, and Director and Founder of the Research and Innovation Center on CO2 and Hydrogen (RICH Center), focused on decarbonization, hydrogen and clean energy, at Khalifa University in Abu Dhabi, United Arab Emirates.

Prof. Vega has developed her career between academia and industry. She obtained her Ph.D. in Physics from the University of Seville, Spain (1992), in collaboration with the Chemical

Engineering Department, University of Southern California, USA where she was a visiting scholar (1990-1992), from where she moved to Cornell University as a Postdoctoral Fellow (1992-1995), before joining Universitat Rovira I Virgili in Tarragona, Spain, where she held several positions in the Chemical Engineering Department and School of Chemical Engineering (1995-2003). In 2003 she moved to the National Research Council of Spain (CSIC), Materials Science Institute of Barcelona, as a Senior Research Scientist, until she joined Air Products in 2007, as the General Director of MATGAS, R&D Director of Carburos Metalicos and Technology Manager of Air Products and Chemicals for CO2, food and water treatment, also leading several projects related to hydrogen. She is the Founder and COE of Alya Technology & Innovation (Alyatech). In 2016 she joined the Petroleum Institute in Abu Dhabi, now part of Khalifa University of Science and Technology as the Joint Chair Professor of the Gas Research Center.

ABSTRACT:

Carbon capture, utilization, and storage and green (or low carbon) hydrogen have been recently identified by the International Energy Agency as two key technologies to decarbonize the energy and industrial sectors. Although most of the captured CO2 would need to be permanently stored, part of it can be converted into value-added products adding economic incentive for CO2 capture while also reducing the environmental footprint of hard-to-abate sectors. Among the CO2 utilization technologies, carbon dioxide reduction reaction (CO2RR) involves converting CO2 into value-added products. This can be done by electrochemical or photocatalytic processes. The main advantages of photocatalytic CO2 conversion versus electrochemical conversion are that it operates at ambient temperatures and pressures and photocatalyst can be designed with high efficiency and tuning selectivity, making it a promising approach for converting solar energy into chemical fuels. Furthermore, the use of hydrogen as a clean and renewable energy source is expected to significantly increase in the foreseeable future, in line with many countries' efforts to compensate for the declining fossil fuel reserves, together with the search for cleaner sources of energy and energy storage at large scale. Hydrogen can be produced by water splitting using electrochemical or photocatalytic processes.

In order to develop and select efficient photocatalysts for CO2 reduction or hydrogen generation (by water or H2S splitting), it is essential, among other features, to understand the interaction of the molecules with catalyst surfaces, mechanism of splitting or conversion, and the limiting barriers; properties that can be provided by quantum methods. After a general introduction, we will showcase the use of DFT for understanding the mechanisms of H2S adsorption and dissociation on CdS surfaces to produce hydrogen, as well as experimental-modeling results on the photocatalytic conversion of gaseous and liquid CO2 on graphene-impregnated Pt/Cu-TiO2, discussing the critical role of Cu dopant. Furthermore, we will present some examples of the use of DFT combined machine learning to guide the selection of efficient photocatalysts for CO2 reduction and hydrogen generation, focused on

a systematic screening of (1) transition-metal-doped Hydroxyapatite for efficient photocatalytic CO2 reduction and (2) transition metal-doped CdS for photocatalytic hydrogen production. The overall objective is to show how computational modeling tools and ML can help to speed up the development of photocatalytic materials for the desired applications.

Hosted by: Prof. Dr. F. Pelayo Garcia de Arquer