



## SEMINARIO

# FROM BULK TO SURFACE MULTIFUNCTIONAL MATERIALS FOR HETEROGENEOUS CATALYSIS CHALLENGES

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From a global point of view, gas phase heterogeneous catalysis (representing *ca.* 90% of all chemical processes) has an enormous impact on the world economy and environmental sustainability. That is why understanding heterogeneous catalysis reactions is one of the central issues of physical chemistry since the past half century. Because the success of a catalytic application begins with catalyst design, it is fundamental to understand the key aspects involved in a catalytic reaction. In that sense a combination of applied catalysis investigations and surface science studies on model catalysts are necessary in order to get this fundamental insight to rationally prepare optimized high surface area catalysts with predefined and controlled bulk and surface properties for specific catalytic applications. In this respect, I will introduce four topics all of them related to the development of multifunctional materials to be used as catalysts for heterogeneous catalysis reactions of high socio-economic and industrial interest. Two different approaches, either applied catalysis or surface science, will be used depending on the specific topic:

1. First of all, I will talk about Mo-V-based mixed metal oxides and their use for partial oxidation of light alkanes as a more sustainable and economic alternative to current petrochemical processes based on olefins.
2. A second topic will focus on nano-structured Au-based catalysts, well known for exhibiting interesting catalytic properties in heterogeneous catalysis reactions at low temperature such as CO selective oxidation or water gas shift reaction (WGS), both key in development of fuel cell technology. A simple but effective strategy to improve their thermal stability (the main drawback of nano-particulate Au catalysts) and so to enhance the scope of use for these materials at higher temperatures will be discussed.
3. The third topic is related to the use of epitaxial graphene as ultimate model catalyst support to prepare superlattices of metal cluster arrays with a very narrow particle size distribution very convenient to study cluster size-dependent activity reactions.
4. Finally, a fundamental study on the interaction of water and CO<sub>2</sub> with a model Fe<sub>3</sub>O<sub>4</sub>(111) surface will be discussed. Conversion of CO<sub>2</sub> into fuels and other value-added chemicals and the use of water as either reaction promoter or hydrogen source for CO<sub>2</sub> reduction/hydrogenation are currently hot topics addressed by obvious environmental and economic motivations widely discussed. Despite advances in this area, further fundamental research needs to be addressed to understand the interaction and behavior of CO<sub>2</sub> and water with catalyst substrates, especially metal-oxide surfaces, in order to rationally design effective heterogeneous catalysts able to carry out such a challenging task.