

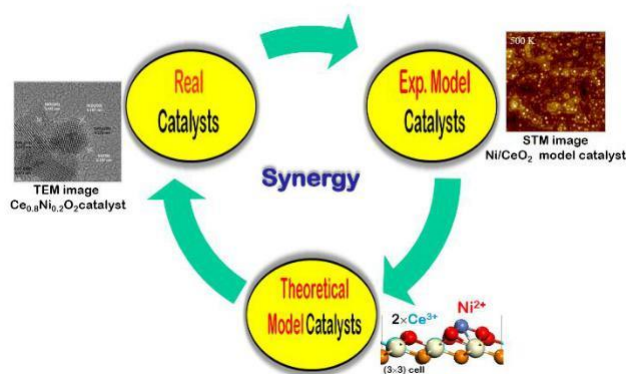
CONTRACT FOR DOCTORAL THESIS

Within the framework of the MICINN 2021 Project PID2021-128915NB-I00

NANOSTRUCTURED CATALYSTS BASED ON CERIUM OXIDE FOR VALORIZATION OF GREENHOUSE GASES

The work combines experimental and theoretical studies and will be carried out at the Institute of Catalysis and Petrochemistry of the Spanish National Research Council, Campus UAM-Cantoblanco under the direction of Dr. M. Verónica Ganduglia-Pirovano and Prof. Arturo Martínez Arias.

The work will focus on the design and characterization of metal-oxide catalysts for the dry reforming reaction of methane with carbon dioxide. CH_4 and CO_2 are two greenhouse gases and their conversion to valuable products is crucial for a cleaner future. To improve existing catalysts and processes for that reaction, it is necessary to improve our knowledge of them from a molecular point of view. The strategy is to study systems as complex as real (powder) catalysts on the one hand and to create and investigate model systems that include essential parts of the real systems, excessively intricate, but which can still be studied at the atomic level by calculations based on the most advanced methods of computational quantum chemistry on the other.



Mild chemical methods (precipitation, microemulsion, hydrothermal) will be used for the preparation of nanostructured systems. The multi-technical structural and chemical characterization data (HREM, XRD, Raman, XAFS, XPS, DRIFTS, EPR, TPR/TPD, textural characterization) will be complemented by studies of the catalysts under reaction conditions using spectroscopic techniques (XPS, XAFS and DRIFTS). The experimental information

obtained will be used as a basis for the theoretical study of model catalysts and the different processes involved in the reactions using first-principles methods based on density functional theory (DFT). The team collaborates with leading national and international laboratories on these issues, both experimental and theoretical.

The announcement is addressed to graduate students, preferably in Chemistry or Physics or Chemical Engineering. A good training in physical chemistry and/or materials science, computational techniques and a good academic record, as well as a Master's degree in the relevant subject areas, will be positively valued.

Interested contact:

Dra. María Verónica Ganduglia-Pirovano
Research Scientist [ORCID: 0000-0003-2408-8898](https://orcid.org/0000-0003-2408-8898)
e-mail: vgp@icp.csic.es
Tel.: +34 91 585 4631
Institute of Catalysis and Petrochemistry (CSIC)
<http://www.icp.csic.es/>
Marie Curie 2, 28049 Madrid

Prof. Arturo Martínez Arias
Research Professor
e-mail: amartinez@icp.csic.es
Tel.: +34 91 585 4940