Two open PhD positions

Two PhD positions in the field of heterogeneous catalysts in the frame of a joint research project between the Instituto de Tecnología Química (CSIC-UPV), the Synchrotron ALBA and the Structure and Chemistry of Nanomaterials Group at Universidad de Cadiz.

The Instituto de Tecnología Química (ITQ) (https://itq.upv-csic.es/en) is an international reference in the field of catalysis and nanostructured materials awarded with the Severo Ochoa Accreditation (2023-2026). The ITQ performs cutting edge research in different disciplines including thermo-, photo- and electro-catalysis equipped with the most modern infrastructure in catalytic processes and spectroscopic characterization.

The synchrotron ALBA (CELLS-ALBA, https://www.cells.es/es) is the Spanish 3-GeV synchrotron radiation facility operated by the Consortium CELLS, which is equally funded by the Spanish Government (Ministerio de Ciencia, Innovación y Universidades) and the Catalan Government (Generalitat de Catalunya, Departament d'Economia i Coneixement). ALBA is a large research infrastructure operating 13 beamlines, complementary facilities, and an Electron Microscopy Center, this last in partnership with other institutions. Currently constructing multiple more beamlines, expanding the Electron Microscopy Center, and integrating advanced data analytics, it sums up a wide range of infrastructures geared toward finding solutions to societal challenges.

The Structure and Chemistry of Nanomaterials Group at Cádiz University (https://fqm334.uca.es) is integrated within the Institute of Electron Microscopy and Materials of this University (IMEYMAT, https://imeymat.uca.es). It counts with access to state-of-the-art facilities for the advanced, atomic scale, characterization of complex, nanostructured, materials for applications in the field of Environmental Catalysis and Catalysis for alternative, green-energy sources. The group has gained an internationally recognized expertise in the development of Transmission and Scanning-Transmission Electron Microscopy methodologies for the ultimate morphological, structural and compositional 2D and 3D characterization of catalysts. The group strongly supports the scientific activities of the Division of Electron Microscopy of Cádiz University (DME-UCA), which is one of the nodes of the Spanish Unique Scientific and Technical Infrastructure (ICTS) of Electron Microscopy of Materials (ELECMI, https://elecmi.es).

The candidate will be mentored by highly qualified experts in the field of heterogeneous catalysis being involved in different research areas oriented to address social challenges. This include i) the synthesis of advanced materials for CO_2 transformation into platform compounds of the chemical Industry, such as alcohols and aldehydes; ii) the catalytic studies including kinetic analysis, and iii) advanced operando spectroscopic studies, getting access to the most modern infrastructures in spectroscopy (synchrotron ALBA) and high resolution microscopy (Universidad de Cadiz).

Dr.P.Concepción (https://scholar.google.es/citations?user=dPr_WgIAAAAJ&hl=es) has wide experience in heterogeneous catalysis and operando spectroscopy. She has been involved in many research projects and collaborations with industry, being co-author of more than 220 publications and 7 patents.

Dr.L.Simonelli (https://scholar.google.com/citations?user=IRbNuegAAAAJ&hl=it) has wide experience in advanced synchrotron based techniques. She focused her research on the study of the interplay between lattice and electronic properties in technologically relevant materials to improve their functionalities. In 20 years of research, she collaborated or leaded several research projects, coauthoring more than 140 publications.

Prof.J.J.Calvino (https://scholar.google.com/citations?hl=es&user=tHqQLusAAAAJ&view_op=list_works&sortby=pubdate) has a strong experience in the atomic scale characterization of nanomaterials using Electron Microscopy based techniques, particularly nanocatalysts. He has coauthored over 250 publications and 5 patents. Likewise, he has been IP of several regional, national and European funded projects.

One PhD offer will be supervised by *Dr.P. Concepción* from the Instituto de Tecnología Química and *Dr.L. Simonelli* from the Synchrotron ALBA. The study will be directed in developing highly active and selective catalyst in the CO_2 activation to target molecules. Catalytic descriptors will be extracted from a correlative catalytic – spectroscopic study, which will be exploited to find out the best catalysts for CO_2 activation and its transformation into alcohols. Interaction with the group of Prof.J.J.Calvino from the University of Cadiz is foreseen for high resolution electron microscopy analysis.

The other PhD will be supervised by *Dr.P. Concepción* from the Instituto de Tecnología Química and *Prof.J.J.Calvino* from the University of Cadiz. The study will be directed in developing highly active and selective catalysts containing single atom, dimers or clusters of controlled atomicity and their study in the CO_2 activation to target molecules. Electron Microscopy techniques will provide direct evidence, with statistical significance, about the atomicity and composition of the active species as well as their spatial distribution and interactions with the support phases. This task will involve the implementation and use of AI tools for data interpretation tasks. Interaction with the group of Dr.L. Simonelli from the Synchrotron ALBA is foreseen for advanced spectroscopic studies.

Reference publications exploiting the multimodal approach allowed by complementary expertise is:

Nature Materials, 2023, 22, 762-768. Development of a highly active Ru based catalyst in the CO_2 hydrogenation to methane at low temperature. The possibility to decrease the reaction temperature from the conventional 350 °C to 180 °C has an important scientific, technological and social impact. The structure of the catalyst and the nature of active sites were characterized by combining advanced imaging and spectroscopic tools at the nano-and macro-scale. *Figure 1* (https://doi.org/10.1038/s41563-023-01540-1)

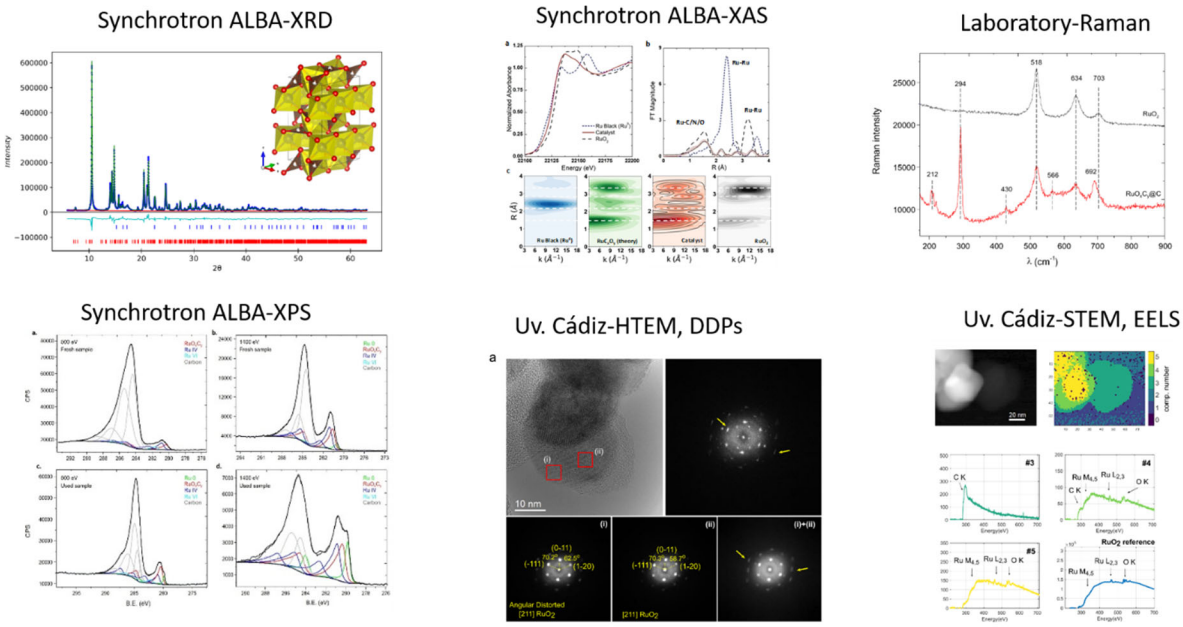


Figure 1, spectroscopic characterization of Ru-based catalyst

Commun Mater 5, 206 (2024). https://doi.org/10.1038/s43246-024-00652-8 . Identification of Pd atoms using Deep Learning methods. *Figure 2.*

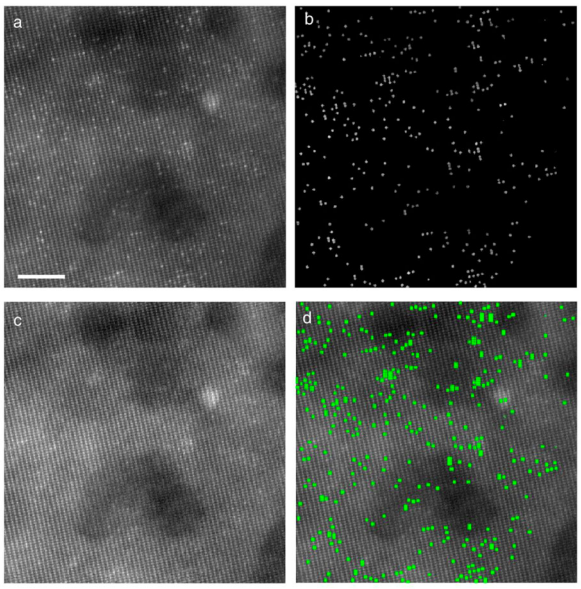
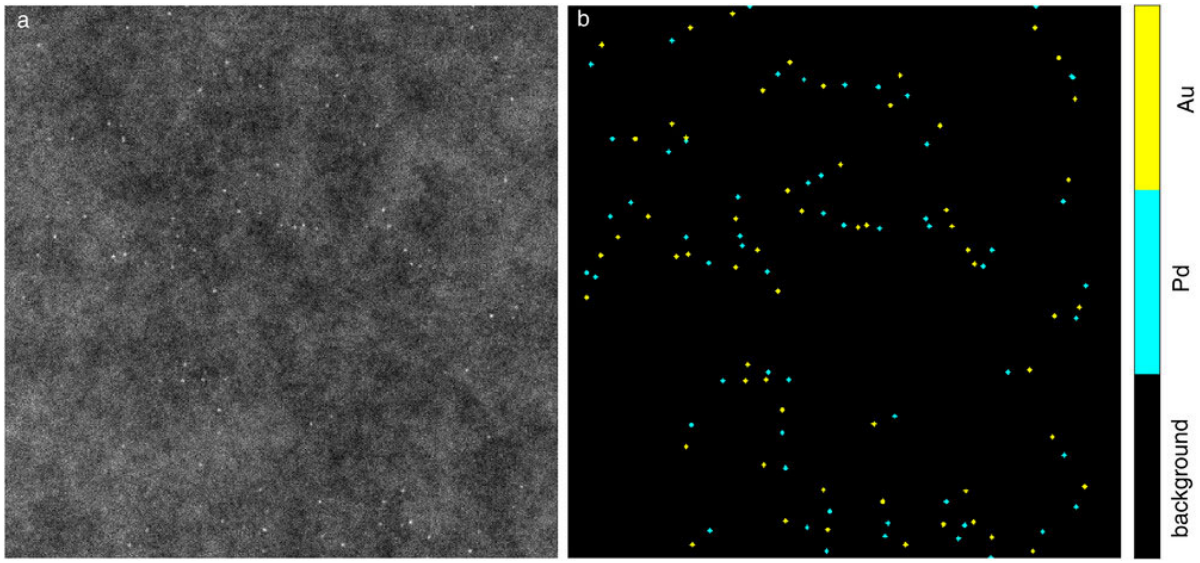


Figure 3. Deep Learning segmentation and in-painting reconstruction. (a) Experimental HR HAADF-STEM image in <211> orientation. (b) Image segmentation of the Pd atoms using Deep Learning methods. (c) Reconstructed HR HAADF-STEM image of the MgO support in <211> zone axis by in-painting methods. Image overlaying Pd pixels in contact with the support. The Pd-cationic column contacts are shown in green and in red those corresponding to Pd-anionic column contacts.

Figure 2. Deep learning segmentation and in-painting reconstruction.

Small Methods 2025, 2402010. https://doi.org/10.1002/smtd.202402010: Experimental HR-HAADF image of PdAu Correlated-SACs on a carbon support (Figure 3, left). Automated segmentation of the image using a specifically trained Neural Network where the chemical nature of the single atoms is determined.



Candidate requirements:

Master degree in Chemistry, Physics or Material Science, with high score (>7).

Highly motivated student with availability to move from one research center to another.

Willingness to learn and acquire new skills.

How to apply

Interested candidates should contact the following researchers: Dr.P. Concepcion (pconcepc@upvnet.upv.es), L.Simonelli (lsimonelli@cells.es) or J.J.Calvino (jose.calvino@gm.uca.es).