

*How nanostructure influences phase composition in metal-oxide catalysts*Elies Molins<sup>1</sup>, Mònica Benito<sup>1</sup>, Ignasi Mata<sup>1</sup><sup>1</sup>Icmab-Csic, Bellaterra, Spain

E-mail: elies.molins@icmab.es

Aerogels are mesoporous materials with high surface areas, which make them specially suited for applications in catalysis [1]. Aerogels for catalysis are initially prepared as amorphous metal-oxide pore structures, and then submitted to calcination for inducing the formation of the active crystalline form. Given the small size of the crystallites formed during the thermal treatment, the aerogel can be considered as formed of nanoparticles. In some cases, smaller, noble metal nanoparticles are attached to the metal-oxide nanoparticles that form the aerogel. Two examples of catalysts for the production of hydrogen from renewable sources are the titania aerogels with gold nanoparticles [2] and zirconia-ceria aerogels [3].

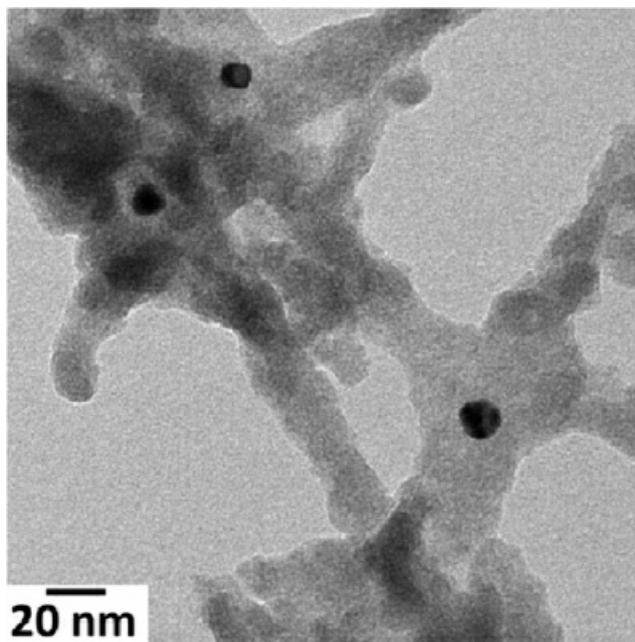
In the case of titania, the fraction of anatase, rutile and amorphous phase determines the catalytic activity of the material. This fraction depends on the parameters of the calcination and on the nanostructure of the aerogel before this calcination, as the stable phase of nanoparticulated titania depends on the size of the nanoparticles. The nanostructure before calcination depends itself on the synthesis route, being influenced by the presence of gold compounds used in the synthesis of the noble metal nanoparticles. A similar situation takes place in the case of ceria-zirconia aerogels, with the added complexity that in this case more phases can be observed as, besides zirconia and ceria in their crystalline or amorphous forms, ceria-zirconia solid solutions of various compositions and different crystal structures can be formed.

Previous results about the relationship between preparation route, nanostructure, phase composition and catalytic properties are presented. In the current study, different routes for the preparation of aerogels are compared, with special attention to the calcination, which is the step that has more influence on the phase composition of the final catalyst. In order to analyze in detail the nanostructure of the catalysts different characterization techniques are used. These include powder X-ray diffraction, including quantitative analysis, for the determination of the phase composition, electron microscopy for obtaining particle size distributions, nitrogen adsorption isotherms for the pore structure and different spectroscopy techniques, which are especially helpful if solid solutions are present. As the objective of this study is the determination of the optimal route for the preparation of catalysts to be used in hydrogen production for feeding fuel cells, the structural characterization is compared with the catalysis results.

[1] Espinal, R. (2012) RSC Adv. 2, 2946-2956.

[2] Murdoch, M. (2011) Nat. Chem. 3, 489-492.

[3] Terribile, D. (1997) Cat. Today 43, 79-88.



**Keywords:** [Hydrogen production](#), [titania aerogel](#), [zirconia-ceria aerogel](#)