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I am pleased to inform you that your contribution **"HYDROGEN STORAGE ON A NOVEL NANOSTRUCTURED CARBON MATERIAL MODIFIED WITH ZIRCONIA"** by *Juliana Maria Juarez, Lisandro F Venosta, Oscar Anunziata, Marcos Bruno Gomez Costa,* has been **accepted** in symposium **A10, Nanostructured Materials and Nanotechnology: Synthesis, Properties, and Theory** at the XXIX International Materials Research Congress, to be held in Cancun in August 15 - 20, 2021.

The presentation has been accepted in the **Poster** modality. Remember that in order to include your abstract in the congress program you must confirm your participation no later than May 21 by choosing the modality you will present your abstract(s); you can do this from your IMRC account.

Organizers of the Symposium
"Nanostructured Materials and Nanotechnology: Synthesis, Properties, and Theory"

Claudia Gutiérrez- Wing, Alfredo Rafael Vilchis Nestor

HYDROGEN STORAGE ON A NOVEL NANOSTRUCTURED CARBON MATERIAL MODIFIED WITH ZIRCONIA

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In this work, we report the synthesis and characterization of zirconium oxide supported in nanostructured carbon material synthesized by a new direct synthesis technique.

The goal of this new method is to avoid the use of inorganic siliceous template (SBA-15), which leads to a shorter and cheaper way to obtain mesoporous carbon, and at the same time incorporate into the framework Zirconium atoms.

The material with zirconium oxide (Zr-CMK-3) was successfully synthesized and characterized by X-ray diffraction, SEM, RAMAN and textural properties, UV-Vis-DRS, X-ray photoelectron spectroscopy and transmission electron microscopy analyses.

Zr-CMK-3 improved significantly the H_2 storage behavior (4.6 wt% at 77 K and 10 bar) compared with CMK-3. The synthesized material is promising for hydrogen uptake by means of weak bonding (physisorption).

The activity of the samples to the adsorption of hydrogen molecules is attributed to the improved dispersion of the zirconium oxide, as well as the appropriate use of support, which can probably disperse the zirconium on its large surface area, allowing a great dispersion of the zirconium.

The Zr^{+4} cation is an active species to absorb and store hydrogen through a physisorption process and the carbon plays an important role in the dispersion and size of metal particles.

A hydrogen storage mechanism on the active surface of the ZrO_2 clusters was proposed. First layer of hydrogen molecules can react with the metal cation through a dihydrogen complex (Kubas interaction). The second layer of hydrogen molecules adsorbed around the metal oxide clusters is due to dipole-like interactions, this is because the metal particle induces dipole forces on the hydrogen molecule. The other layers could also interact by dipole forces; however, the interaction force decreases as the distance to the surface increases. The upper layers could interact with the metal cation by dipole-induced bonding; however, the interaction force decreases as the distance to the surface increases.

Keywords: CMK-3, HYDROGEN STORAGE, ZIRCONIA

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