

Direct Synthesis and characterization of mesoporous carbon CMK-3 modified with zirconia applied in energy storage

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In this work, we report the synthesis and characterization of the nanostructured carbon material (CMK-3) modified with zirconium oxide synthesized by a new direct synthesis technique.

The aim of this new synthesis 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.

Zirconium oxide dispersed in carbon materials (Zr-CMK-3) were successfully synthesized and characterized by X-ray diffraction, textural properties, UV-Vis-DRS, XPS, and transmission electron microscopy analysis.

This material is promising in the application of hydrogen adsorption for energy storage. Zr-CMK-3 material significantly improved H₂ storage behavior (4.6% by weight at 77 K and 10 bar) compared to CMK-3 support. The synthesized material is promising in the absorption of hydrogen by weak bonding forces (physisorption). A hydrogen adsorption mechanism was proposed and the role of the Zr⁺⁴ cation in hydrogen absorption was discussed.

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 ZrO₂ clusters was proposed.

First layer of hydrogen molecules can react with the metal cation through a dihydrogen complex (Kubas interaction) [1]. 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 interaction of the induced dipole in a second layer adsorbs more hydrogen molecules because the strong interaction of the metal particles takes up dipole-induced forces on the hydrogen molecules. 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.

The procedure for this adsorption is still under investigation and optimization. The hydrogen storage behavior in Zr-CMK-3 can be optimized by controlling the size of the metal particles, the dispersion and the nature of the support.

[1] Y. Takasu, R. Unwin, B. Tesche, A.M. Bradshaw, M. Grunze Surf. Sci. 77 (1978) 219.