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ANM2021 Abstract Acceptance Notification- 344

Para: oanunziata@frc.utn.edu.ar

Dear Oscar A. Anunziata,

Thank you for your work entitled “New Method for CMK-3 Synthesis Modified with Zr Applied in H2 Storage” submitted to ANM2021 Portugal (22-24 July 2021, Aveiro, Portugal).

We are pleased to inform you that your abstract (ID 344) is accepted for **Oral** presentation in session of HE (Hydrogen Energy) at ANM2021 conference.

Kindly confirm your **Physical or Virtual** participation by registering at https://www.congressospco.abreu.pt/ANM2020-37888.aspx

The schedule of your presentation will be emailed to you by 15 June 2021.

Please visit the conference website ANM2021 Portugal for conference updates.

Best Regards,

Dr. Elby Titus (On behalf of ANM2021 conference chairs)

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New Method for CMK-3 Synthesis Modified with Zr Applied in H_2 Storage

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INTRODUCTION

In this work we develop a novel direct synthesis method of modified CMK-3 with zirconium oxide. This modification occurs during the synthesis process. Our assessment includes a one-step synthesis of nanostructured mesoporous carbon modified with zirconium oxide, the characterization of the resulting material by XRD, N2 adsorption, XPS, UV-Vis, TEM, SEM and Raman. We show the enhancement of the storage capacity of the composite material, compared to bare CMK-3.

EXPERIMENTAL

The silica source (TEOS) is added along with the other components in a one-step synthesis. Sucrose ($C_{12}H_{22}O_{11}$) was used as a carbon precursor and Zirconium Oxychloride (Cl_2OZr x 8 H_2O) as a zirconium source. The sol-gel polimerization of silica with Pluronic P123 surfactant and sucrose, yields a composite silica/P123/sucrose. This composite is further treated with sulfuric acid and then carbonized. Finally, the ordered mesoporous carbon (OMC) is obtained by removing the silica template.

RESULTS AND DISCUSSION

XRD shows that Zr-CMK-3 can be associated with a hexagonal crystallographic structure of the P6mm group. The zirconium-modified carbon mesoporous material has a high surface area of 820 m^2/g and a pore diameter of 6.5 nm. The synthesized material was also characterized by Raman spectroscopy, showing the characteristic first-order bands of a carbonaceous material, normalized to the G-band intensity. For further information about the Zirconium modified CMK-3 material structure and pore size, TEM studies were performed. Fig.1 indicates a distinctively visible ordered pore arrangement, characteristic of CMK-3 structure [1]. The pore size is in the range of 6-7 nm, in good agreement with the average pore sizes calculated by the QSDFT model.

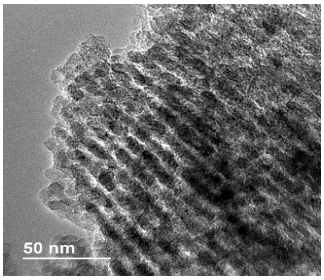

Fig. 1 TEM Image of Zr-CMK-3

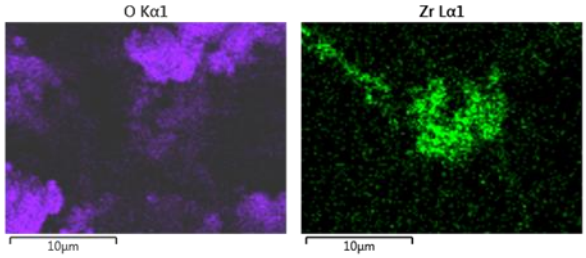

Fig. 2 SEM-EDX of Zr-CMK-3

Figure 2 shows SEM and EDX images Zr-CMK-3, can be seen mainly Zr and O.

The XPS spectra (Fig. 3a) of, C-ZrO2 show the $3d_{5/2}$ and $3d_{3/2}$ spin-orbit splitting doublet located at 184 and 186 eV, respectively. This suggests that the chemical environment of Zr4+ has changed after being supported on the CMK-3 nanomaterial, in agreement with that reported by Juan [2]. The hydrogen storage behavior in Zr-CMK-3 can be optimized by controlling the size of the metallic particles, dispersion and the structure of the support (Fig.3b)

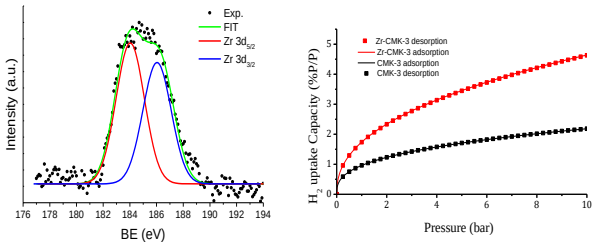

Fig. 3: (a) XPS of Zr and, (b) H_2 uptake of Zr-CMK-3

CONCLUSION

A novel ordered mesoporous carbon was obtained by direct synthesis and it was decorated with zirconium oxide. The synthesized materials show promise in fully reversible weak bond strength in hydrogen adsorption

REFERENCES

1. J. Juarez, M. Gomez, O. Anunziata., J. Por Mat 25, 1359 – 1363 (2018).
2. J. Juan JC, et al., Mat Res Bull 42, 1278–1285 (2007).

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