

Workshop Summary
ALBA II - Workshop on present and future perspectives of catalysis

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<i>Speaker</i>	<i>Date</i>
Joaquin Silvestre Albero	01/07/2021

Speaker and team:

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Title: "Structural flexibility in MOFs upon gas adsorption"

Short Abstract:

One of the main issues when working with metal-organic framework (MOF) materials concerns the presence of structural changes upon an external stimulus (e.g., upon variations in pressure and/or temperature). These structural dynamics are crucial to understand their performance in a given application, e.g., gas adsorption/separation processes, reaction conditions, etc. Structural changes in MOFs include gate-opening and/or breathing phenomena, phase transitions, among others. In this project, we have used MSPD station at the ALBA synchrotron to evaluate the structural characteristics of MOFs under operando conditions. These studies have been performed in several zeolitic-imidazole frameworks (ZIFs) with unusual adsorption performance (e.g., ZIF-7, ZIF-4, etc.). In-situ studies at the synchrotron have been crucial to identify and understand this "anomalous" adsorption performance through the identification of the structural details and their perturbation under operando conditions.

Describe the technique/probe to solve the grand challenge (about 1500 characters):

To evaluate the structural changes taking place upon adsorption we have used the MSPD station at the ALBA synchrotron facilities. Experiments were performed in a thin capillary containing a given amount of ZIF and connected on-line to a gas dosing system. Experiments were performed at different temperatures and after dosing different concentrations of the target molecule. The combination of temperature and pressure changes allowed us to identify the response of the evaluated ZIFs towards external stimuli, and the crystallographic changes associated.

Provide supporting literature, if appropriate or necessary:

C. Cuadrado-Collados, J. Fernandez-Catala, F. Fauth, Y.Q. Cheng, L.L. Daemen, A.J. Ramirez-Cuesta, J. Silvestre-Albero, Understanding the breathing phenomena in nano-ZIF-7 upon gas adsorption, J. Mater. Chem. A 5 (2017) 20938.

J. Gandara-Loe, A. Missyul, F. Fauth, L.L. Daemen, Y.Q. Cheng, A.J. Ramirez-Cuesta, P.I. Ravikovitch, J. Silvestre-Albero, New insights into the breathing phenomenon in ZIF-4, *J. Mater. Chem. A* 7 (2019) 14552.

C. Cuadrado-Collados, G. Mouchaham, L. Daemen, Y. Cheng, A. Ramirez-Cuesta, H. Aggarwal, A. Missyul, M. Eddaoudi, Y. Belmabkhout, J. Silvestre-Albero, Quest for an optimal methane hydrate formation in the pores of hydrolytically stable metal-organic frameworks, *J. Am. Chem. Soc.* 142 (2020) 13391-13397.

J. Gandara-Loe, R. Bueno-Perez, A. Missyul, D. Fairen-Jimenez, J. Silvestre-Albero, Molecular sieving properties of nanoporous mixed-linker ZIF-62: Associated structural changes upon gas adsorption application, *ACS Appl. Nano Mater.* 4 (2021) 3519-3528.