

Experimental report

14/02/2025

Proposal: INTER-589

Council: 10/2023

Title: Evaluating the potentials of Zr-C4MOF for DAC of hydrophobic greenhouse gases

Research area:

This proposal is a new proposal

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Experimental team:

Local contacts: Monica JIMENEZ RUIZ

Samples: Based-MOF fcu Topology, C₂₄H₁₆O₃₂Zr₆

Instrument	Requested days	Allocated days	From	To
IN1 LAG	3	3	16/11/2023	19/11/2023

Abstract:

Evaluating the potentials of Zr-C4 MOFs for DAC of hydrophobic greenhouse gases

In this experiment was measured the MOF-808 conformed by $\text{Zr}_6\text{O}_4(\text{OH})_4$ clusters connected to six formate (HCOO^-)₆ ligands providing the MOF-808 secondary build unit (SBU) $\text{Zr}_6\text{O}_4(\text{OH})_4(\text{HCOO}^-)_{12}$. Each SBU is bound through 1,3,5-benzenetricarboxylate (BTC^{3-}) linkers, producing the well-known building blocks of the MOF-808 $\text{Zr}_6\text{O}_4(\text{OH})_4(\text{BTC}^{3-})_2(\text{HCOO}^-)_6$. It was studied the effect of MOF-808 functionalization with the aminoacids arginine and lysine in the adsorption of CO_2 . The measurements of INS were divided in two parts: (1) the ones for the MOF-808, Lys, Arg, MOF-808@Lys⁺, and MOF-808@Arg⁺ (see Fig. 1(a) and (b)); (2) the ones for the loaded systems MOF-808@Lys⁺+CO₂ and MOF-808@Arg⁺+CO₂ (see Fig. 1(c) and (d)). The sample masses utilized were 1.4376 g of MOF-808, 1.5643 g of Lys, 1.5124 g of Arg, 1.3876 g of MOF-808@Lys, and 1.7214 g of MOF-808@Arg. The purpose to measure the MOF-808, Lys, and Arg was to identify the new bands that the aminoacids inclusion could produce in the hybrid systems MOF@Aminoacid. It was used 1 bar of CO₂ for the experiments of the loaded samples. It was utilized the monochromator Cu(220) to capture energy transfers of $E_i = 85\text{--}223$ meV ($k_i = 650\text{--}1800$ cm⁻¹) with an energy resolution of $\Delta E/E = 2\%$. All measurements were done at 10 K for both empty and gassed MOFs, using aluminum sample holders, which were also measured empty.

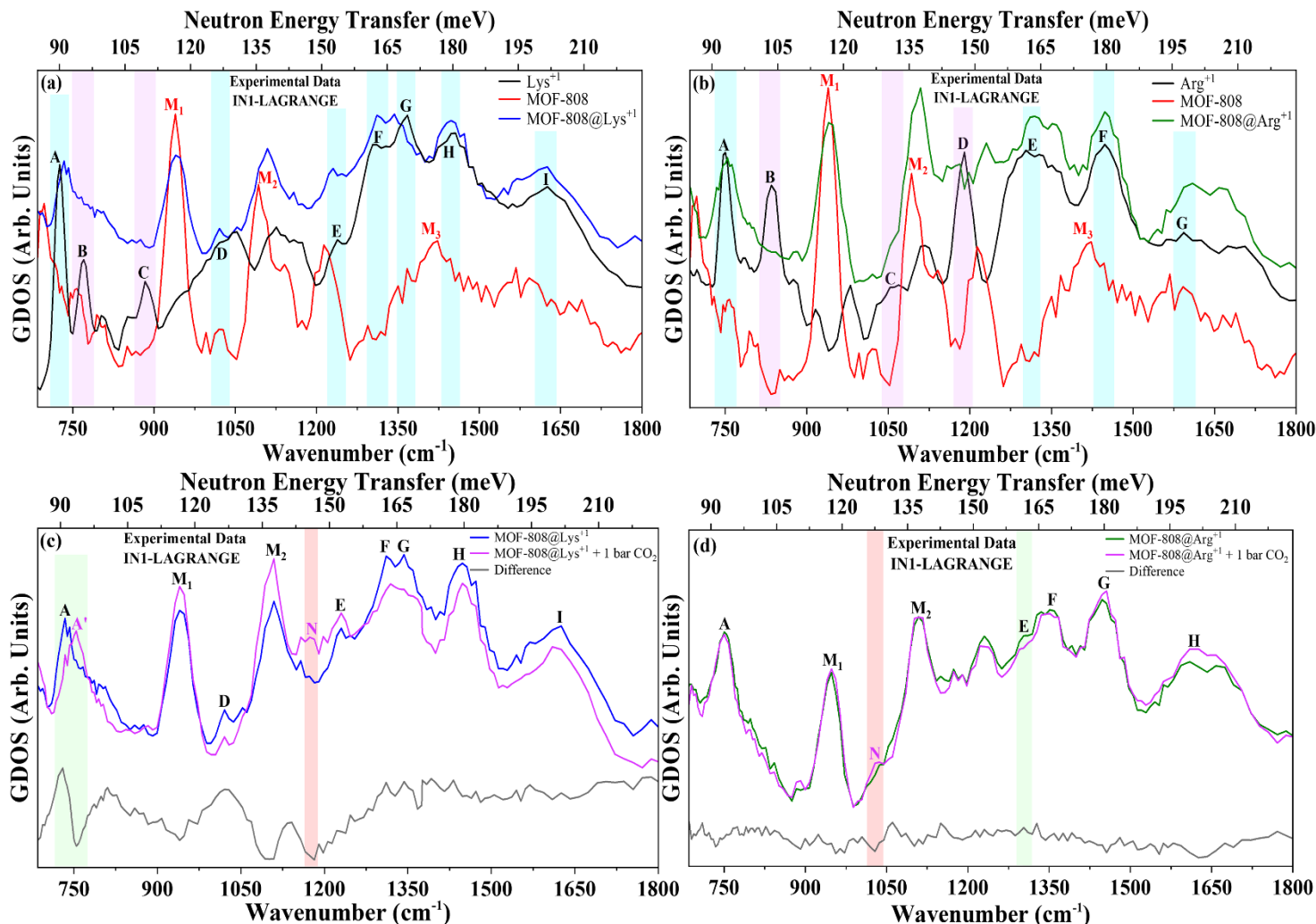


Figure 1: (a) INS spectra for Lys⁺, MOF-808, and MOF-808@Lys⁺; (b) INS spectra for Arg⁺, MOF-808, and MOF-808@Arg⁺; (c) INS spectra for the unloaded MOF-808@Lys⁺ and for that one loaded with 1 bar of CO₂; (d) INS spectra for the unloaded MOF-808@Arg⁺ and for that one loaded with 1 bar of CO₂.