INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON



Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	Experiment title: Development of a serie of Al-V- bimetallic metal organic frameworks	Experiment number: 26-01-1046
Beamline:	Date of experiment:	Date of report:
BM26A	from: 20/02/2016 to: 25/02/2016	
Shifts:	Local contact(s):	Received at ESRF:
15	Dipanjan Banerjee	
Names and affiliations of applicants (* indicates experimentalists): Karen Leus ¹ , Hannes Depauw ¹ , Irena Nevjestic ² , Pieter Tack ³ , Stephen Bauters ³ , Laszlo Vincze ³ , Pascal Van Der Voort ¹		
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[°] Department of Analytical Chemistry, Ghent University		

Report:

Paper published: Wang, G. *et al.* Enhanced gas sorption and breathing properties of the new sulfone functionalized COMOC-2 metal organic framework. *Dalton transactions* **45**, 9485-9491, doi:10.1039/c6dt01355d (2016).

Abstract: A new sulfone functionalized vanadium metal-organic framework (MOF), denoted as SO2-COMOC-2, has been synthesized solvothermally. Its structural and gas sorption properties towards CO2 and CH4 have been evaluated and compared to those of the pristine COMOC-2 material. The SO2-COMOC-2 shows a remarkable increase in CO2 capacity at ambient pressure (2.13 mmol g(-1) at 273 K vs. 1.23 mmol g(-1) for the pristine COMOC-2). Additionally, the high pressure CO2 sorption isotherm shows a distinctive two-step sorption behavior with a final capacity of 12.45 mmol g(-1) for SO2-COMOC-2 at 303 K, while for CH4 a typical Type I isotherm was obtained with a capacity of 4.13 mmol g(-1). In situ synchrotron X-ray powder diffraction measurements have been carried out to characterize the structural flexibility of the materials, showing both the presence of large pore and narrow pore form. Furthermore, synchrotron XANES and a variety of spectroscopic techniques have been utilized to verify the presence of hydroxyl groups and the existence of the mixed vanadium oxidation states in the titled MOF structure.