



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://www.esrf.fr/misapps/SMISWebClient/protected/welcome.do>

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal (“relevant report”)

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a “*preliminary report*”),
- even for experiments whose scientific area is different from the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as “relevant report(s)” in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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.



	Experiment title: Unveiling the evolution of atomically dispersed Mn species supported on TiO ₂ for NO Selective Reduction Reaction with NH ₃	Experiment number: A30-2-1160
Beamline: BM 30	Date of experiment: from: 8 th November 2022 to: 14 th November 2022	Date of report:
Shifts: 18	Local contact(s): Antonio Aguilar Abdallah Nassereddine	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): <i>Yan Wang, Cristina Queiros da Silva*, Sarah Komaty Zaarour*, Sudheesh Kumar Veeranmaril*, Javier Ruiz-Martinez</i> KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology, Thuwal, Saudi Arabia		

Report:

Observing catalysis behavior at atomic level for Mn sites can bring better understanding of its role towards NH₃-SCR of NO. Herein, we prepared a series of highly dispersed MnOx/TiO₂ via impregnation method. Based on our laboratory characterizations (XRD, HRTEM, HAADF-STM and Easy-XAFS), no nanoparticle was observed, however we cannot further confirm cluster or single atom which contributed to the performance. To resolve this puzzle, tracking molecularity and oxidation state of Mn at real time by operando XAS is the best option. Hence, we applied the beamline experiment and finished the study. Concerning the structural characterization, XAS spectra has been recorded at Mn K-edge (6.5 keV). The fluorescence detection available on BM30 beamline (Canberra 13 elements) successfully provided high quality EXAFS spectra for all metal loadings.

This ESRF experiment (A30-2-1160) was successfully performed, the atomically dispersed Mn species structures were confirmed by XAS, seen the Figure a, which could be very crucial for our current research. Besides, the operando XAS measurement (Figure b) further verified that Mn single atom exhibited excellent NH₃-SCR catalytic performance under different real working conditions over MnOx/TiO₂, which were also

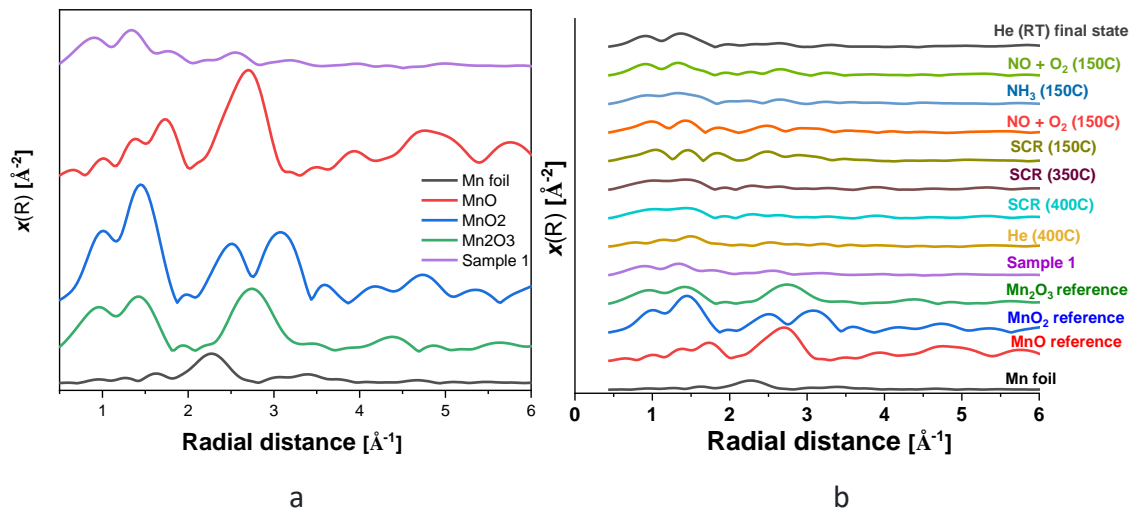


Figure a) Mn K edge EXAFS spectra of sample 1 and references. b) Operando Mn K edge EXAFS spectra of sample 1 under SCR conditions.

observed in our lab. This study will provide new insight towards relationship between structure and performance at atomic level for designing superior NH_3 -SCR catalysts.

The qualitative assessments provided in this report will be completed by a thorough analysis of the ensemble of XAS spectra and by a publication.

