

<b>Coach</b> Valentijn De Coster	<b>Supervisor(s)</b> Vladimir V. Galvita Hilde Poelman	<b>Funding</b>
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## Analyzing Big Data: MEXAS on Ni-Fe Methane Dry Reforming Catalysts

### Aim

Apply big data analysis tools to analyze modulation-excitation X-ray absorption spectroscopy (MEXAS) data of Ni-Fe methane dry reforming (DRM) catalysts to gain insight into the electronic and structural dynamics of Ni and Fe under DRM conditions.

### Justification

CO<sub>2</sub> utilization is a must to achieve the climate goals set for the current century. In this regard, Ni-Fe catalysts for methane dry reforming ( $\text{CO}_2 + \text{CH}_4 \leftrightarrow 2\text{CO} + 2\text{H}_2$ ) show great promise: they combine the high activity intrinsic to Ni with the carbon-resistant behavior of Fe materials and are cost-effective alternatives to their noble metal-based counterparts [1]. To improve the

design of these catalysts, studies are required to understand their behavior under reactive conditions. For this purpose, *in situ/operando* quick-XAS (QXAS) with ~s time resolution is an interesting tool, as it yields element-specific electronic and structural information. Moreover, when combined with periodic modulations of the reaction environment, this results in so-called MEXAS [2] experiments (Figure 1) which help to elucidate the presence of short-lived intermediates within the catalytic material.

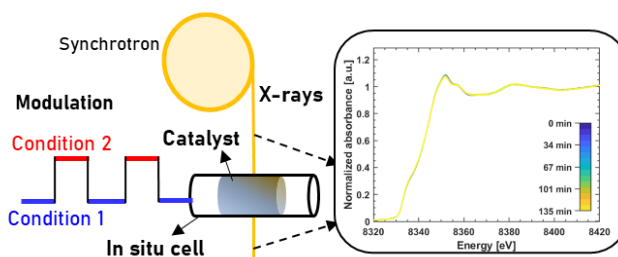


Figure 1. Schematic representation of MEXAS experiments.

However, MEXAS (and QXAS in general) typically yields large data volumes that require dedicated tools to analyze them efficiently. Therefore, building on the LCT's in-house expertise in both 'standard' (EXAFS modelling) and 'big data' (PCA, MCR-ALS) (Q)XAS analysis tools [3], this project will focus on the examination of MEXAS data acquired for Ni-Fe catalysts under cycling DRM conditions to resolve the electronic and structural changes that occur for Ni and Fe during DRM.

### Program

1. Literature survey on Ni-Fe DRM catalysts, MEXAS, conventional (EXAFS modelling) and big data (Q)XAS analysis tools (PCA, MCR-ALS).
2. Application of big data analysis tools to MEXAS data obtained for Ni-Fe DRM catalysts.
3. Combine results from big data analysis tools with conventional XAS data analysis (e.g. EXAFS modelling) to assist the interpretation of big data results.

[1] S.A. Theofanidis, V.V. Galvita, H. Poelman, G.B. Marin, Enhanced Carbon-Resistant Dry Reforming Fe-Ni Catalyst: Role of Fe, *ACS Catal.* 5 (2015) 3028-3039.

[2] D. Ferri, M.A. Newton, M. Nachtegaal, Modulation Excitation X-Ray Absorption Spectroscopy to Probe Surface Species on Heterogeneous Catalysts, *Topics in Catalysis* 54 (2011) 1070.

[3] V. De Coster, N.V. Srinath, S.A. Theofanidis, L. Pirro, A. Van Alboom, H. Poelman, M.K. Sabbe, G.B. Marin, V.V. Galvita, Looking inside a Ni-Fe/MgAl<sub>2</sub>O<sub>4</sub> catalyst for methane dry reforming via Mössbauer spectroscopy and in situ QXAS, *Appl. Catal. B: Environ.* 300 (2022) 120720.