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Analyzing Big Data: Modulation-excitation X-ray Absorption Spectroscopy of 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_2 utilization is a must to achieve the climate goals set for the current century. In this regard, Ni-Fe catalysts for methane dry reforming ($CO_2 + CH_4 \leftrightarrow 2CO + 2H_2$) show great promise: they combine the high activity intrinsic to Ni with the carbon-resistant behavior of Fe materials and provide 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 (**Error! Reference source not found.**) which help to elucidate the presence of short-lived intermediates within the catalytic material. This latter is achieved by subjecting the collected time-resolved data to phase-sensitive detection (PSD), yielding phase-resolved spectra which represent only the active surface fraction of the catalyst which responded to the applied modulations. Thus, MEXAS-PSD allows for surface-sensitive QXAS measurements, a trait which is absent in 'conventional' QXAS experiments.

However, MEXAS 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[3-4], 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.

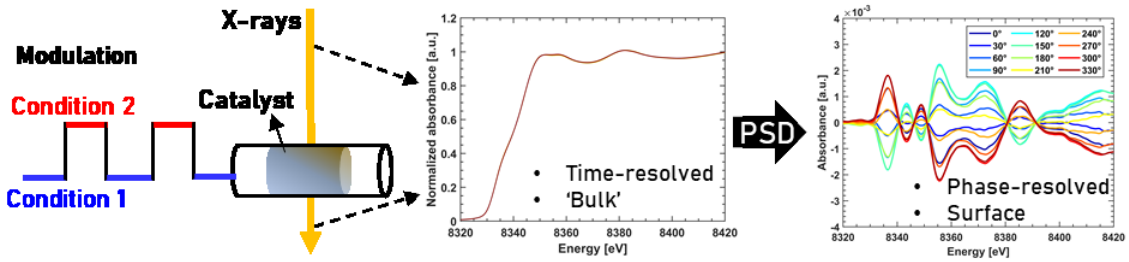

Figure 1. Schematic representation of MEXAS experiments with a posteriori PSD analysis.

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.

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2. Ferri, D.; Newton, M. A.; Nachtegaal, M., *Top. Catal.* **2011,** 54 (16), 1070.
3. De Coster, V.; Srinath, N. V.; Theofanidis, S. A.; Pirro, L.; Van Alboom, A.; Poelman, H.; Sabbe, M. K.; Marin, G. B.; Galvita, V. V., *Appl. Catal. B: Environ.* **2022,** 300, 120720.
4. De Coster, V.; Srinath, N. V.; Yazdani, P.; Poelman, H.; Galvita, V. V., *J. Phys. Chem. Lett.* **2022**, 7947-7952.