**Data overview: Modulation Engineering: Stimulation Design for Enhanced Kinetic Information from Modulation-Excitation Experiments on Catalytic Systems**

<https://zenodo.org/records/7780501>

This document is an overview of the attached dataset.   
(QXAS = quick X-ray absorption spectroscopy)

**.txt files**

* *norm\_Fe\_YYY\_av2000\_00001.txt (YYY = Fe\_foil, Fe2O3\_pellet, Fe3O4\_pellet, FeO\_pellet, G-Fe2O3\_ref, Ni\_foil, NiO)*  
  Normalized (“norm”) Fe K edge or Ni K edge QXAS data of reference materials YYY, recorded at room temperature, obtained by averaging over 2000 consecutive scans (“av2000”)
* *norm\_Fe\_Ni-MgFeAlO4\_AsPrepared.txt, norm\_Ni\_Ni-MgFeAlO4\_AsPrepared*  
  Normalized Fe K edge (“\_Fe\_”) and Ni K edge (“\_Ni\_”) QXAS data recorded at room temperature of as prepared Ni/MgFeAlO4, recorded at room temperature, obtained by averaging over 2000 consecutive scans (“av2000”)
* *norm\_Fe\_Ni-MgFeAlO4\_postTPR.txt, norm\_Fe\_Ni-MgFeAlO4\_postTPR.txt*Normalized Fe K edge (“\_Fe\_”) and Ni K edge (“\_Ni\_”) QXAS data recorded at room temperature of recuded Ni/MgFeAlO4, recorded at room temperature, obtained by averaging over 2000 consecutive scans (“av2000”)
* *Ni3Fe\_Spectrum\_Normalized.nor*Normalized Fe K edge XAS spectrum of a Ni3Fe alloy reference
* *XRD\_MgFeAlO4.dat, XRD\_Ni-MgFeAlO4.dat*X-ray diffraction (XRD) patterns of as prepared MgFeAlO4 and Ni/MgFeAlO4

**.7z files – In situ QXAS data**

* *Fe\_Blank\_MEXAS\_RT\_normalized.7z, Ni\_Blank\_MEXAS\_RT\_normalized.7z*  
  Normalized Fe K edge (“\_Fe\_”) and Ni K edge (“\_Ni\_”) QXAS data recorded during a blank He modulation-excitation experiment, recorded at room temperature.  
  Each spectrum within is a normalized .txt file (cfr. the “norm\_” files above”)
* *Fe\_Ni-MgFeAlO4\_TPR\_normalized.7z, Ni\_Ni-MgFeAlO4\_TPR\_normalized.7z*Normalized Fe K edge (“\_Fe\_”) and Ni K edge (“\_Ni\_”) QXAS data recorded during H2 temperature-programmed reduction of Ni/MgFeAlO4.
* Fe\_Ni-MgFeAlO4\_MEXAS\_normalized.7z, Ni\_Ni-MgFeAlO4\_MEXAS\_normalized.7z  
  Normalized Fe K edge (“\_Fe\_”) and Ni K edge (“\_Ni\_”) QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4.

**.mat files (MATLAB)**

* *Flows\_Blank\_MEXAS.mat*Recorded flows of H2, He, CO2, and calculated partial pressures, applied during a blank He modulation-excitation program.
* *Fe\_MCRResultsTt\_10Ni10Fe\_TPR\_2PIES.mat, Ni\_MCRResultsTt\_10Ni10Fe\_TPR\_2PIES.mat*Results of multivariate curve resolution-alternating least-squares (MCR-ALS) analysis applied to Fe (“Fe\_”) and Ni (“Ni\_”) K edge QXAS data recorded during H2-TPR of as prepared Ni/MgFeAlO4.
* FrequencyAnalysis\_Blank\_MEXAS.mat  
  Frequency analysis of the He partial pressures applied during a blank He modulation-excitation program.
* *Flows\_Pressures\_MEXAS.mat*Recorded flows of H2, He, CO2, and calculated partial pressures, applied during a H2/CO2 modulation-excitation program of activated Ni/MgFeAlO4.
* *FrequencyAnalysis\_Modulation.mat*Frequency analysis of the H2, He and CO2 partial pressures applied during a H2/CO2 modulation-excitation program of activated Ni/MgFeAlO4program.
* *MCRRes\_MEXAS\_Fe.mat, MCRRes\_MEXAS\_Ni.mat*Results of MCR-ALS applied to Fe (“\_Fe”) and Ni (“\_Ni”) K edge QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4.
* *FrequencyAnalysis\_MEXAS\_Fe.mat, FrequencyAnalysis\_MEXAS\_Ni.mat*Frequency analysis results of the MCR-ALS results of Fe (“\_Fe”) and Ni (“\_Ni”) K edge QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4.
* *PSDdata\_Fe\_Blank\_MEXAS.mat, PSDdata\_Ni\_Blank\_MEXAS.mat*Phase-sensitive detection (PSD) results of Fe (“\_Fe”) and Ni (“\_Ni”) K edge QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4.
* *PSDdata\_Fe\_k1.mat, PSDdata\_Fe\_k2*PSD results of Fe K edge data QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4, obtained with demodulation index 1 (“\_k1”) and 2 (“\_k2”).
* *PSDdata\_Ni.mat*PSD results of Ni K edge data QXAS data recorded during modulation-excitation of reduced Ni/MgFeAlO4.