Implementation of an Automated Evaluation for an Quantitative Analysis of Mass Spectrometer Data

The path to a climate-neutral future: methanol steam reforming using perovskite oxides

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Perovskites & Exsolution

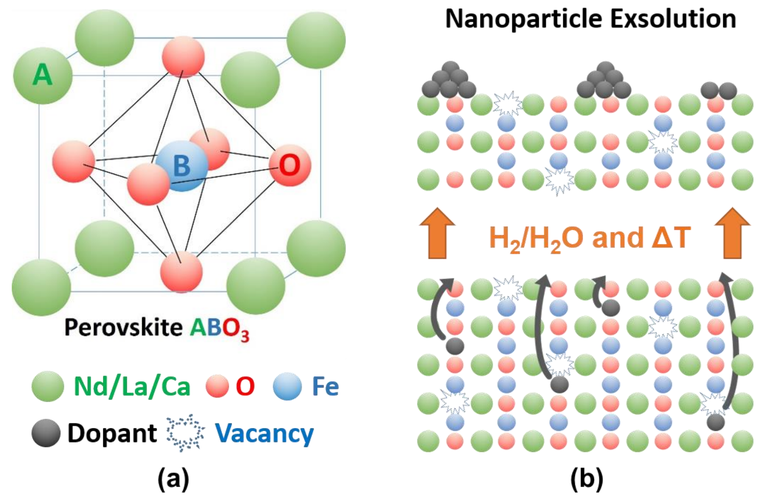
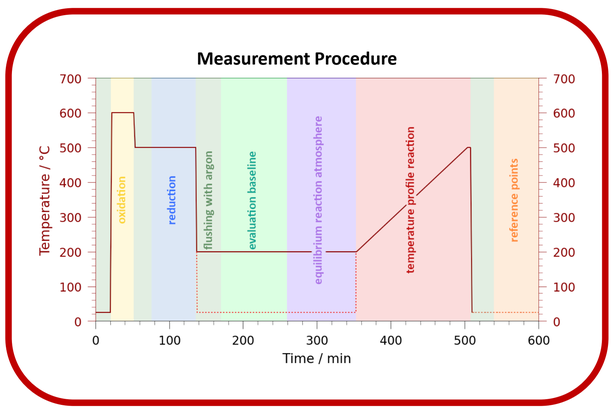


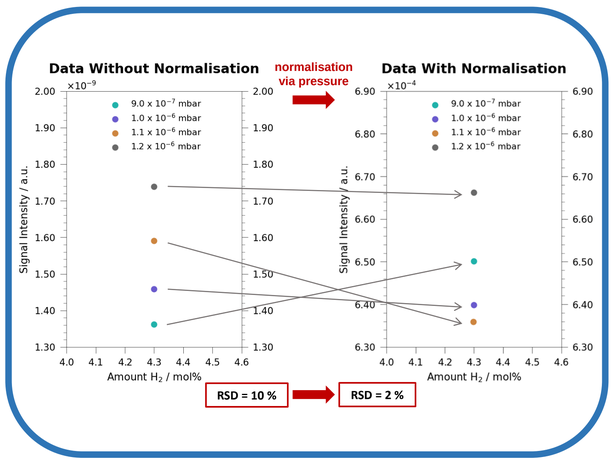
***Figure 1** – Perovskite*
***a)** Illustration of a perovskite-type oxide with the formula ABO_3. In green: A-site cation, in blue: B-site cation and in **red**: oxygen. Doping of the respective sites is possible. **b)** Formation of catalytically active nanoparticles on the surface of the material. During the reduction of the material, oxygen vacancies are formed, leading to nucleation. Due to diffusion of exsolvable metal ions, nanoparticle growth takes place on the surface.*

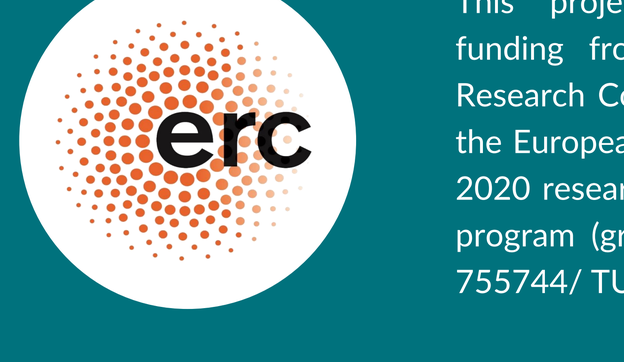
Introduction

Methanol Steam Reforming (**MSR**) with the reaction formula: $H_2O + CH_3OH \rightleftharpoons CO_2 + 3\ H_2$ provides a promising solution for the **on-demand production of hydrogen.** Due to **high reaction temperatures** and possible **side reactions,** the use of proper catalysts is of crucial importance.[1] Promising materials are **perovskite-type oxides** which show an outstanding property called **exsolution**.[2] Due to the water saturated gas atmosphere, a **calibration strategy** for a mass spectrometer (MS) was implemented. To standardise the evaluation procedure for future applications, a **python toolkit** was developed in the course of this work.

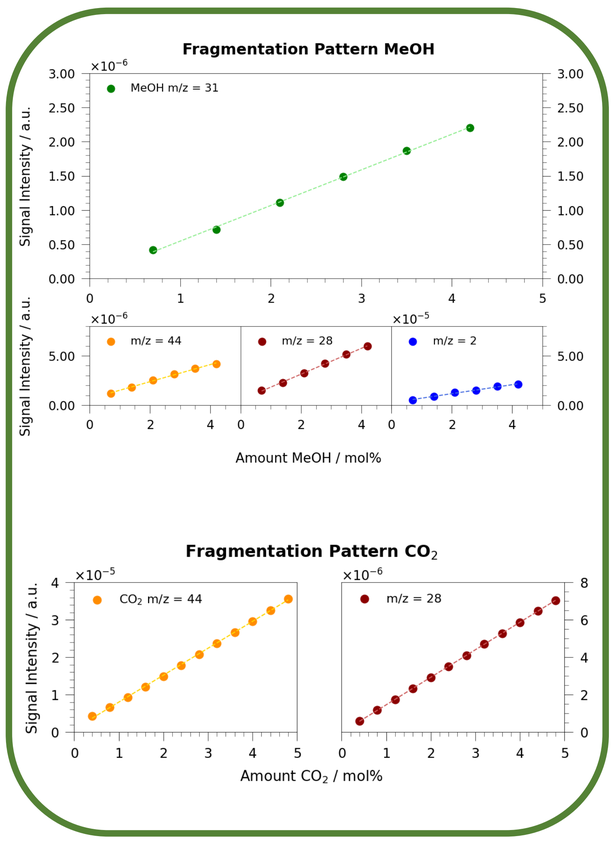
Python Toolkit

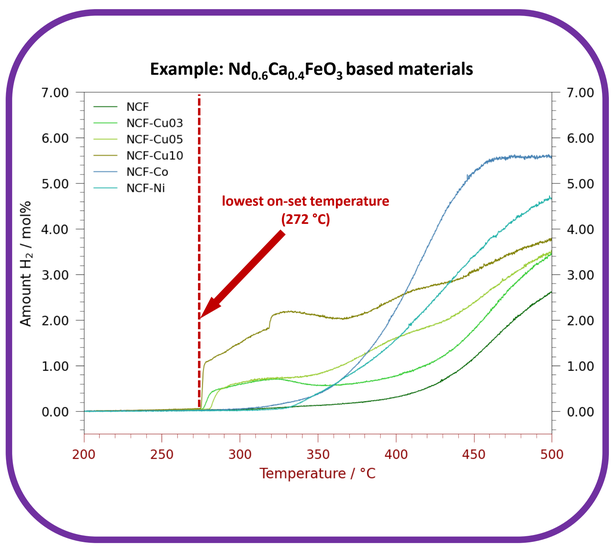







```
def program data_evaluation

# several steps are necessary for the quantitative analysis of MS data
# implementation of defined measurement procedure
## 1. Data Import ------------------------------------------------------------
# necessary files: MS data (rawdata), recorded temperature, calibration information


## 2. Normalisation of Data using recorded Pressure --------------------------
# normalisation of raw data using the recorded working pressure
# to eliminate pressure dependency of signal intensities and reduce RSD of data
      for all signals:
            normalized_data = rawdata/pressure


## 3. Correction of Baseline -------------------------------------------------
# search for individual baseline of the respective signals after the reduction period
# start of baseline indicated by a stable signal of m/z ratio of 2 (hydrogen)
      if stable signal found:
            start calculation mean value of baseline of individual signals
            subtract mean value from normalized_data


## 4. Calculation of Methanol Amount -----------------------------------------
# amount of methanol necessary for the evaluation of formed fragments
# used as starting point for the correction process of fragmentation
      for data points of signal_MeOH:
            amount_MeOH = (y(signal_MeOH)-d(calibration_MeOH)/k(calibration_MeOH)


## 5. Correction of Raw Data using Fragmentation Pattern ---------------------
# correction of rawdata according to obtained fragmentation patterns of CO2 and MeOH
      for data points of signal_CO2, signal_CO and signal_H2:
            correct data according to fragmentation patterns using amount_MeOH
# calculation amount of CO2 for correction of CO and H2 signals via CO2 fragments
      for data points of signal_CO2:
            amount_CO2 = (y(signal_CO2)-d(calibration_CO2)/k(calibration_CO2)
      for data points of signal_CO and signal_H2:
            correct data according to fragmentation patterns using amount_CO2


## 6. Example Results of Analysis --------------------------------------------
# automated plot of gas composition, selectivity, specific activity and yield
      save all data in dataframe
      plot results for amount of H2

end program data_evaluation
```





Outlook

After implementing a reliable procedure for the **quantitative analysis of mass spectrometer data**, further investigations of the most promising materials regarding their catalytic activity towards **MSR** are going to be performed.

References

[1] T. A. Rocha, F. Ibanhi, F. Colmati, J. J. Linares, V. A. Paganin, and E. R. Gonzalez, J. Appl. Electrochem., vol. 43, no. 8, pp. 817–827, Aug. 2013.

[2] L. Lindenthal, R. Rameshan, H. Summerer, T. Ruh, J. Popovic, A. Nenning, S. Löffler, A. Opitz, P. Blaha and C. Rameshan, Catalysts, vol. 10, no. 3, Art. no. 3, pp. 268-281, Mar. 2020.

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