AI-supported and automated data analysis

of electrocatalytic CO_2 capture and conversion

Master 2 internship project

Location: Laboratoire de Chimie et Biologie des Métaux (LCBM)

Duration: 4 months

Supervisor : Dr Laurent Sévery (laurent.severy@cea.fr)

Objectives & Project

Data analysis is critical in experimental fields, as both statistics and variation reflect the reality of experimentally collected data. This is particularly true and relevant for the field of electrocatalysis (the science and technology at stake to produce e-fuels and e-chemicals from renewable resources), where complex systems and measurements are convoluted into a small number of observable or measured values, making rigorous data analysis essential to uncover underlying phenomena. With the rise of automated experimentation, AI-driven analysis becomes critical to handle high-dimensional data, identify hidden correlations, and guide experimental optimization.

This internship, embedded in the "AUDACE! Air Capture" project, focuses on coupled CO_2 capture and valorization using molecular catalysts immobilized on carbon nanotube and solution capture agents. It combines retrospective data analysis, AI-assisted optimization, and tool development with the following concrete aims:

1. Data Analysis & Automated Data Analysis Tools
    - Process cyclic voltammetry (CV) and chronoamperometry data coupled with chromatographic analysis under varied CO_2 capture & conversion conditions.
    - Design scalable Python scripts for automated processing of electrochemical and chromatographic data, compatible with diverse acquisition formats
2. AI-Assisted Optimization & Validation
    - Develop predictive models to explain experimental observations and identify key performance drivers.
    - Use machine learning (e.g., regression, clustering, Bayesian optimization) to:
        - Extract catalytic system fingerprints from existing datasets.
        - Propose optimized experimental conditions (e.g., electrolyte, potential, catalyst loading) for improved CO_2 capture efficiency and conversion selectivity.
    - Test AI-generated hypotheses experimentally in collaboration with the team.

The expected outcomes are the following:

- Automated pipelines for electrochemical/chromatographic data processing.
- AI models for electrocatalytic system analysis and condition optimization.
- Experimental validation of optimized CO_2 capture/valorization conditions.