## Project 2:

# On the catalytic pyrolysis mechanisms of plastic model compounds

#### Motivation:

By 2015, approximately 6 billion metric tons of plastic waste had been produced, and projections suggest a potential increase to 26 billion metric tons by 2050 if current growth rates continue. The low rate of plastic waste upcycling, currently below 10%, raises concerns regarding the achievement of a sustainable and circular society. Catalytic pyrolysis holds promise for converting plastic waste into valuable chemicals and fuels, but its complex chemistry, including challenges like side reactions such as coking, must be addressed.

#### **Objective:**

This project aims to achieve a thorough understanding of plastic pyrolysis mechanisms using operando photoelectron photoion coincidence (PEPICO) spectroscopy. By employing vacuum ultraviolet (VUV) synchrotron radiation, PEPICO has proven to be a versatile tool for detecting reactive intermediates in catalysis, combustion, and pyrolysis. [1,2] Through this combination of mass spectrometry and threshold photoelectron spectroscopy, the complex reaction mechanism can be comprehended. Understanding the underlying chemistry may lead to a more targeted optimization of the catalytic pyrolysis process for the production of valuable products from waste plastic in the future.

#### Your task:

You will be carrying out initial measurements in a catalytic pyrolysis GC/MS setup at ETH to explore a selection of catalysts and model compounds relevant for plastic pyrolysis. The best performing ones will be subjected to reactions under very controlled conditions in a catalytic microreactor utilizing molecular beams to unveil the decomposition pathways at the SOLEIL synchrotron (France). In addition to mass spectrometry, threshold photoelectron spectroscopy will be employed as an isomer-selective technique to determine the structure of the products and reactive intermediates, including radicals. This data will lead to a comprehensive understanding of the catalytic plastic pyrolysis process, revealing the role of the structure and active sites of the catalyst.

#### Timeframe:

October 2023 – February 2024: Beamtime at the Soleil Synchrotron scheduled for November 28 – December 3rd.

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#### **Reference:**

<sup>[1]</sup>*Catal. Sci.* **2020**, 10, 1975-1990. <sup>[2]</sup>*Energy Fuels* **2021**, 35, 16265–16302.