

Project 1:

On the 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:

By subjecting specific plastic model compounds, e.g., from polyvinyl chloride (PVC), to controlled conditions in a hot microreactor using molecular beam techniques, the decomposition pathways can be fully explored using synchrotron radiation from the Swiss Light Source (SLS). 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. To gain a comprehensive understanding of the pyrolysis process, quantum chemical calculations using advanced computational packages (Gaussian 16) will be conducted to obtain a detailed potential energy surface.

Timeframe:

September 2023 - January 2024: Beamtime at the SLS scheduled for September 10-14.

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Reference:

[1] *Catal. Sci.* **2020**, 10, 1975-1990.

[2] *Energy Fuels* **2021**, 35, 16265–16302.