TITLE OF PROJECT

Project title:	Event-averaged and time-resolved ambient-pressure XPS as a new tool to study catalysis.
PRISMAS Research Area:	Clean Energy
Supervisor:	Jan Knudsen
Hosting University:	Lund University

1. Project summary:

Understanding the atomic level behaviour of working catalytic surfaces is a key challenge for design of novel catalysts. Even for what appears to be steady state conditions, the catalyst structure and chemical composition – and thus reactivity and specificity – fluctuates in time in response to the instantaneous gas-mixture, pressure and temperature. Therefore, methods that can access the temporal behaviour of a catalytic system with ms-µs time-resolution during ongoing reactions must be established.
In this PhD project we will develop advanced instrumentation and methods for time-resolved in-situ measurements of catalyst materials using gas-composition, pressure, and temperature pulse pertubations. Combining this methodology with ambient pressure x-ray and ultraviolet photoelectron spectroscopy we will focus on bimetallic transition metal surfaces and particles and study reactions ranging from CO oxidation to CO_2 hydrogenation.

2. Keywords (up to 5)

APXPS
Catalysis
Time-resolved
XPS
UPS

3. Project outline

- State of the art:

Recently, we developed in situ methodologies and instrumentation capable of measuring the chemical state of a catalyst surface and the localized gas composition above it– including product molecules formed - simultaneously and with ms to µs time-resolution (See Knudsen et al., Nature Communications 12, 6117 (2021), Shavorskiy et al., ACS Applied Materials & Interfaces, 13, 40 (2021), Shavorskiy et al., Synchrotron Radiation News, 35, 4-10 (2022)). Very recently, we developed a new measurement scheme capable of distinguishing between active and spectator phases on catalyst surfaces at operando conditions.

Co-funded by the European Union

- Project objectives:

In this PhD project we will develop and improve photoelectron spectroscopy instrumentation and methodology for advanced time-resolved and event-averaged in situ measurements of catalyst surfaces exposed to cyclic gas composition or temperature pulses. Subsequently, we will use the new instrumentation and methodology to study structural oscillations on catalyst surfaces with high time-resolution and link this to catalyst function. Altogether, this gives a unique possibility both to reveal short-lived species or phases and distinguishing active and spectator phases on the catalyst surface, which is impossible to do with conventional APXPS. For the project we plan to focus on bimetallic transition metal surfaces and particles and study reactions ranging from CO oxidation to CO_2 hydrogenation. The methods and instrumentation developed in this project will significantly improve the possibilities at the APXPS beamlines at MAX IV and currently we are working actively to transferred new methodology beyond APXPS.

- References:

Knudsen et al., Nature Communications 12, 6117 (2021)
Shavorskiy et al., ACS Applied Materials & Interfaces, 13, 40 (2021)
Shavorskiy et al., Synchrotron Radiation News, 35, 4-10 (2022)

4. Link to job application

- Link to job application: Apply here
- Link to PRISMAS overview: https://www.maxiv.lu.se/prismas/