

Catalysis enabled by *operando* spectroscopy: from fundamental understanding to innovative materials

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Heterogeneous catalysis is of prominent importance for modern society. For example, the Fe catalysed NH₃ synthesis process provides nitrogen fertilizers that lead to food production for at least half of the world's population. It is even more important in the circular economy, providing process solutions for future energy conversion, fuel production, and waste recycling. Yet the understanding of reaction mechanisms is still limited due to the complexity of surface catalytic systems and the lack of characterization methods to directly observe surface process under working conditions.

In this talk, I will introduce new experimental designs to utilize synchrotron X-rays and X-ray free electron laser-based *operando* spectroscopy to identify active centres and rate determine steps, which leads to the development and synthesis of novel materials that have significantly improved catalytic performance. I will present recent method development in my group:

1. Measuring the half reaction rate to determine rate limiting steps in catalysis.
2. Measuring bond energy upon the formation of oxygen vacancies.
3. Measuring dynamics of elementary electron transfer from support to metal active site at fs to ps time scale, help to shoot the molecular movie of a single catalytic process.

With these first-time observations, we have been able to develop new catalysts with 5-100 times better performances than those in existing reports for emission control, H₂ production, and fuel cell applications. Our new *operando* X-ray methods have been used beyond catalysis to energy storage and conversion systems. Such innovation has great potential in wide engineering applications.