



## UK Catalysis Hub X-ray Spectroscopy Simulation for Understanding Catalysts Workshop

**10 April 2026**

Meeting Room M1&2, Research Complex at Harwell, Rutherford Appleton Laboratory,  
Harwell Campus, Didcot, OX11 0QX

### Programme

10:00 - 10:30	Registration Tea & Coffee
<b>SESSION 1</b>	<b>CHAIR:</b> <i>Dr. Simon Kondrat, Loughborough University</i>
10:30 – 10:40	<b>Welcome &amp; introduction</b> Dr. Simon Kondrat, Loughborough University
10:40 – 11:15	<b>Theory &amp; simulations of XAS, XPS and RIXS</b> Prof. Dr. Frank de Groot, Utrecht University
11:15 – 11:50	<b>Seeing Surface Species Differently: A New Operando Picture of Ammonia Decomposition Catalysts</b> Dr. Liqun Kang, Max Planck Institute for Chemical Energy Conversion
11:50 – 12:25	<b>Title TBD</b> Dr. Luke Higgins, Diamond Light Source
12:25 – 12:45	<b>Discussion (20 mins) Led by Dr. Simon Kondrat</b>
12:45 – 13:30	<b>LUNCH</b>
<b>SESSION 2</b>	<b>CHAIR:</b> <i>Dr. Mark Isaacs, University College London</i>
13:00 – 14:05	<b>Using theory to support hard X-ray spectroscopy at Diamond</b> Dr. Joshua Elliott, Diamond Light Source
14:05 – 14:40	<b>X-ray photoelectron spectroscopy - progress and challenges for electronic structure theory</b> Prof. Anna Regoutz, University of Oxford
14:40 – 15:15	<b>X-Ray Absorption and RIXS on Coordination Complexes</b> Dr. Michael Baker, University of Manchester ( <i>remote</i> )
15:15 - 15:35	<b>BREAK</b>
15:35 - 16:10	<b>XAS as Process Analytical Technology (PAT): Towards Real-Time Online XANES/NEXAFS Analysis</b> Prof. Sven Schroeder, University of Leeds ( <i>remote</i> )
16:10 - 16:30	<b>Discussion (20 mins) Led by Dr. Mark Isaacs</b>
16.30	<b>Close</b>