



Contribution ID: 2

Type: **not specified**

Simulation and Fitting of the Operando GISAXS data in BornAgain: A Case of Catalytically Active Supported Metal Nanoparticles

Wednesday, 19 December 2018 17:45 (15 minutes)

Our group is employing a combination of the surface-sensitive methods such as Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) and Grazing-Incidence X-ray Diffraction (GIXD) to follow structural evolution in a series of catalytically active supported metal nanoparticles (NPs) on the flat single crystal substrates in real time under industrially relevant conditions. [1, 2]. By fitting the GISAXS data in the BornAgain [3] package it was demonstrated that supported Au NPs undergo size and shape transformations during CO oxidation [1] reaction, primarily due to gold oxide removal at the metal-support interface along the particle perimeter. Our results support the dual catalytic sites mechanism whereby CO is activated on the gold surface whereas molecular oxygen is dissociating at the gold-support interface. The GISAXS data analysis and fitting including a choice of the structural model and minimization algorithms will be discussed in detail. To show versatility of the method the preliminary results on the surface-related changes in the cobalt NPs during Fischer-Tropsch synthesis will be also presented.

Title

Primary author: ODARCHENKO, Yaroslav (University College London)

Presenter: ODARCHENKO, Yaroslav (University College London)

Session Classification: User session