Unraveling Complex Surface Reaction Pathways Using Soft X-ray Spectroscopy

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Ceria catalysts are commonly used in many fuel related processes such as the Water-gas-shift reaction, alcohol reforming, and fuel cell applications. We have been systematically examining the adsorption and reaction of various oxygenated hydrocarbons as these functionalized molecules provide fundamental building blocks for understanding the reactions of more complex biomass materials. C 1s and O 1s core-level photoelectron spectroscopy are used to identify various chemical intermediates on the surface. Near-edge x-ray absorption spectroscopy is also used to differentiate between similar species that may or may not have unsaturated bonds. Specific unique examples include the formation of dioxymethylene, $O\text{-}CH_2\text{-}O$, from formaldehyde as indicated by the C 1s peak position and the absence of a C=O resonance in the NEXAFS spectrum. In addition various C_2-oxygenates form ethylenolate, $\text{-}O\text{-}CH{=}CH_2$, as indicated by the alkyl and alcohol peaks in the C 1s sXPS and a C=C resonance in the C k-edge NEXAFS.

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