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The Active Phase of Gold Catalyst for Propylene Epoxidation

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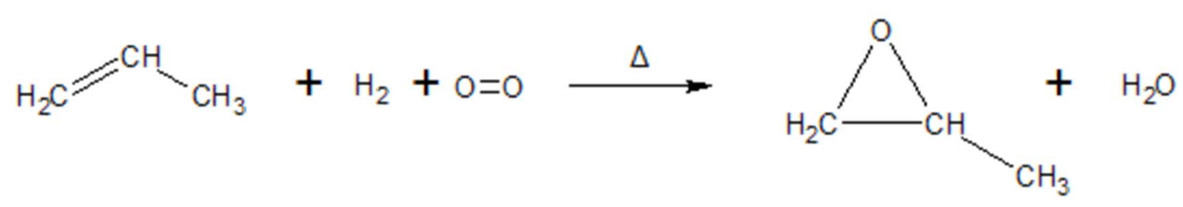
Introduction



- Propylene Oxide (PO) is an important chemical intermediate which is used in production of polyurethane foams, resins, polyethers and propylene glycol.
- Traditional method involves chlorohydrin and other organic hydro peroxides; It involves multiple steps and additional separation and purification units which makes the process more costly.
- The method of direct propylene epoxidation with molecular H_2 and O_2 converting to PO is more simpler and better for the environment.
- Gold supported on titania-on-silica ($Au/TiO_2/SiO_2$) and Gold supported on titanosilicalite (Au/TS-1) catalysts were tested to improve the production of PO.
- The purpose of this research was to use X-ray Absorption Spectroscopy (XAS) technique to analyze the data.

X-ray Absorption Spectroscopy (XAS)

- XAS is an inner shell spectroscopy where an x-ray interacts with core electron.
  - XANES - X-ray Absorption Near Edge Spectroscopy
    - It refers to the neighboring region of the absorption edge of XAS measurement (pre-edge, edge, near edge)
  - EXAFS - Extended X-ray Absorption Fine Structure
    - It is the oscillatory data extending hundreds of volts above the edge

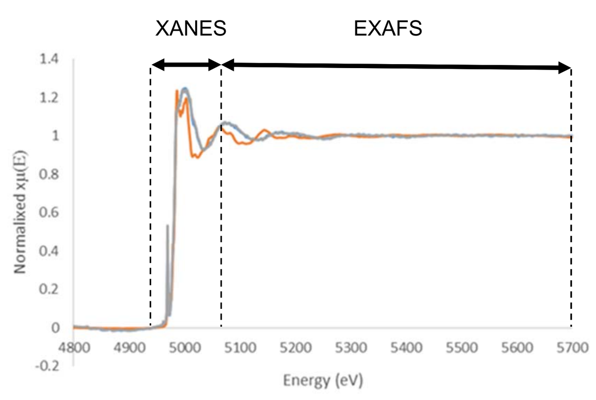


Figure1. Regions of XAS

APS/ANL

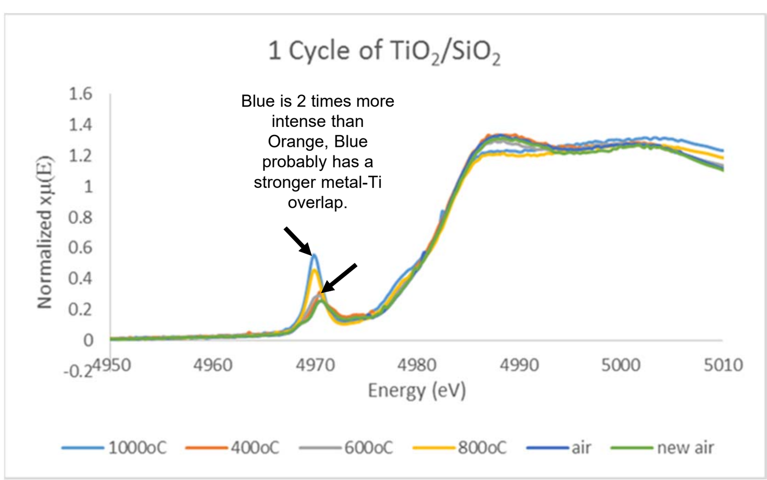
- APS – Advanced Photon Source
- ANL – Argonne National Laboratory (Chicago)
- Beamline 9 – It provides intense and tunable x-ray beams for XANES experiments

Figure 2. Location of the Experiment

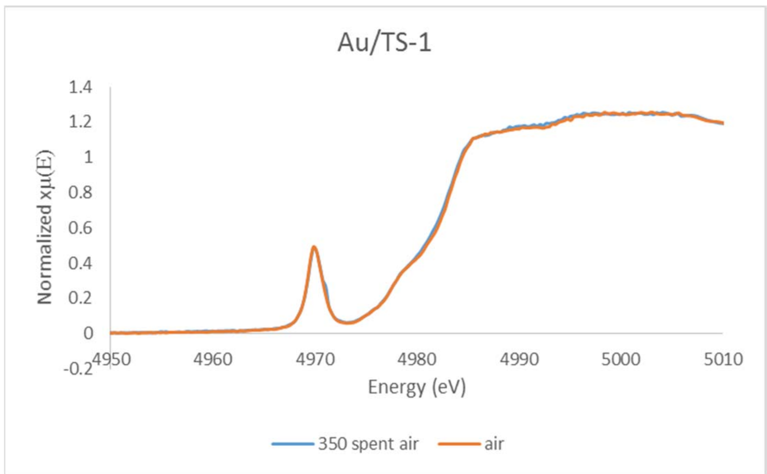
Ti K Edge

Figure 3: The XANES regions of Au on TiO_2 on SiO_2 at varying temperatures form 400ºC to 1000ºC (A) and Au on TS-1 (B) are shown.

- When temperature was increased, the titania-on-silica-supported catalyst resulted in higher pre-edge intensity at 4970 eV (A).
- Change in peaks (A) showed that the coordination number of Ti4+ decrease from 6 towards 4 which favors PO formation.
- The exact overlap of both trials of Au/TS-1 (B) showed no change in coordination number of Ti4+.



A



B

Au L3 Edge

- Figure 4: Au/TS-1 catalyst was tested at various temperatures.
- The sample was tested with increase in temperature (25ºC – 300ºC) and again at 200ºC.
- Dropping the temperature back did not affect the results; no change was seen here.
- Gold remained as metallic gold under reaction conditions (H_2 + O_2 + C_3H_6 at 200ºC).

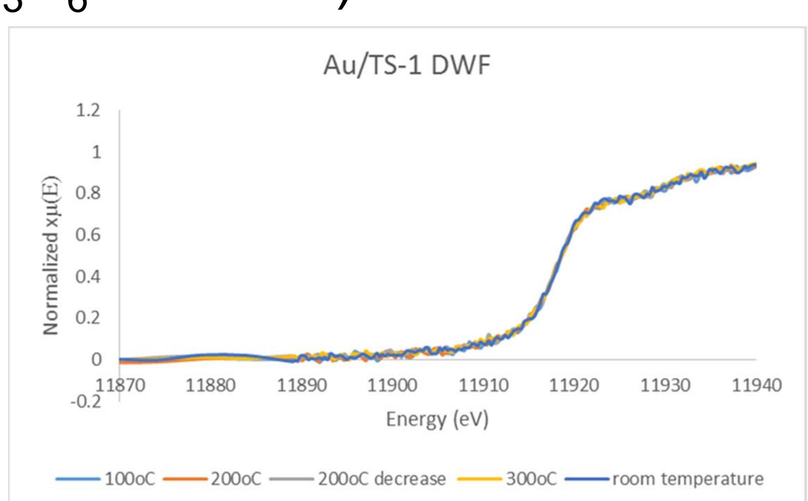


Figure 4. XANES region of Au/TS-1 catalyst of L3 Edge

Conclusions

- More efficient method of producing propylene oxide was examined, through propylene epoxidation with molecular H_2 and O_2.
- $Au/TiO_2/SiO_2$ and Au/TS-1 catalysts were chosen for this experiment.
- X-ray Absorption Spectroscopy analysis showed increasing the temperature (A) led to a lower coordination number of Ti4+ favoring PO formation; also no changes were seen in Au metal at 200ºC.

Acknowledgments

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