At the National Synchrotron Light Source at Brookhaven NIST, Dow Scientists Reveal Catalysts' Private Lives

What do car interiors, adhesives, and sterilizing agents have in common? They are all produced from propylene oxide, a volatile, colorless liquid with a $10 billion-annual market value.

At the NSLS, scientists who work for the National Institute of Standards & Technology (NIST) in Gaithersburg, Maryland, and Dow Chemical in Midland, Michigan, are studying how to produce propylene oxide in a single-step, environmentally friendly way.

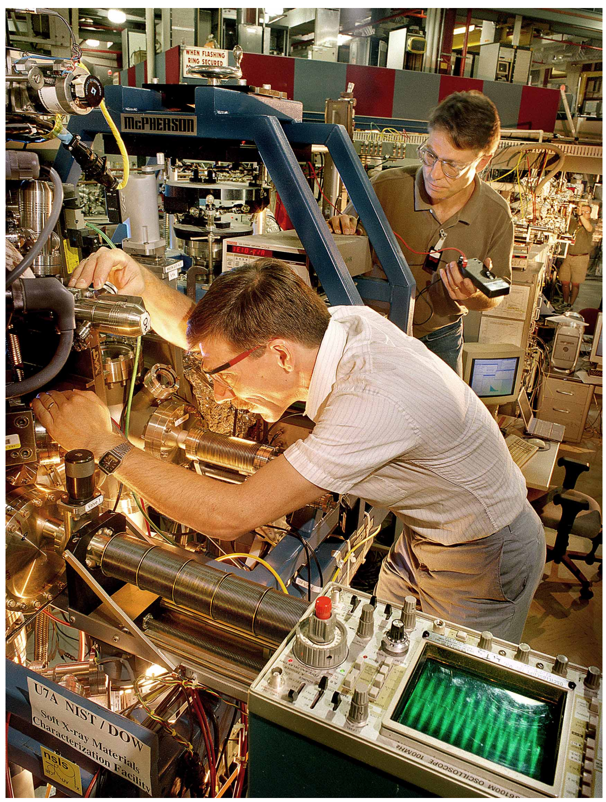
To help in their investigations, they have designed and built a state-of-the-art instrument that is now producing very exciting results.

Propylene oxide is produced by combining propylene, a flammable gas obtained by breaking up petroleum molecules, with oxygen. The process is accelerated by chemicals which act as catalysts.

"Selecting the best catalysts is usually done by testing different chemicals and choosing the one with the best results," says Daniel Fischer, NIST physicist and team leader. "Instead, we are developing a new method that reveals the complex transformations that occur during a chemical reaction. With that knowledge, we may be able to develop cleaner and more efficient catalysts for propylene oxidation."

To study the role of two types of catalysts, platinum on alumina and zeolites, which are cage-like molecules, Fischer and his colleagues use a technique called near-edge x-ray absorption fine structure (NEXAFS).

In NEXAFS, very intense x-rays are projected toward a cell containing the reactants and the catalyst. By precisely tuning the wavelength or "color" of the x-rays, the scientists select x-rays with low-energy, soft x-rays, which probe every step of the chemical reaction.



At the National Synchrotron Light Source, National Institute of Standards & Technology's Dan Fischer (front) and former Dow Chemical chemist Simon Bare prepare equipment for a catalysis experiment.

The soft x-rays are scattered or re-emitted by the chemicals, then analyzed by a detector. The detector produces a spectrum of signals, each providing information on the chemical bonds between the atoms present in the reactants and the catalyst.

"The signals act like fingerprints," says Fischer. "You can watch bonds form and break as the signals wax and wane with time. It is like looking inside a black box, the eyes being the detector and the synchrotron radiation providing the illumination."

Getting clearly separated signals, however, was not easy. When the scientists first looked at their NEXAFS spectra six years ago, the signals of interest were camouflaged by many others.

So Fischer and NIST postdoc Sharadha Sambasivan developed and refined an instrument that would filter the x-rays coming off the reaction cell by reflecting the desirable x-rays and absorbing the others. The instrument, called a normal incidence focusing multi-layer mirror, is a state-of-the-art device that dramatically reduces the background.

"The originality of this work is in being able to understand how these reactants and catalysts work together under real conditions," Fischer says. "Now we have the tools to really find out what is going on at the atomic level in catalysts at work to catch a glimpse of their private lives!"

-Patrice Pages

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