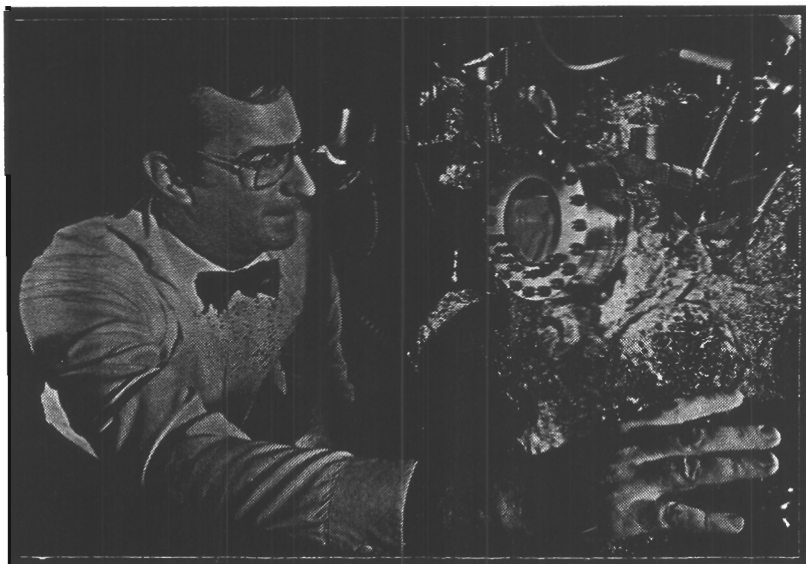


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CREATING "DESIGNER CATALYSTS": RESEARCHERS LINK METAL OXIDE STRUCTURES WITH EFFECTS ON CHEMICAL REACTIONS, REDUCE TRIAL AND ERROR

Choosing or creating a metal oxide catalyst to drive a chemical reaction is usually a labor-intensive process involving trial and error. Researchers at the Georgia Institute of Technology have found a way to make the process more certain and specific by studying the links between the structure of catalysts and their effects on reactions, said Associate Professor Mark G. White.

"You can decide what properties you want to produce, and, by inference, we can tell you what type of catalytic structure you need to obtain them," said White, Director of Georgia Tech's Focused Research Program in Surface Science and Catalysis.



Dr. Mark White adjusts surface science equipment in the lab of Dr. H. P. Gillis, School of Chemistry. (Color Slides/B&W Prints Available)

"We are showing unambiguous relationships between structure and catalytic properties."

Presented Tuesday, August 25 at the American Chemical Society's annual meeting in Washington, D.C., the research has a variety of potential applications. Catalysts could be developed for use in everything from cleaning flue gases and manufacturing plastics to creating protective clothing for firefighters, soldiers and environmental cleanup specialists.

The key to this work has been the creation of single layers of special metal-containing catalytic molecules on a ceramic oxide surface. The researchers synthesize metal complexes using nucleophilic groups present as ligands -- particles that form a "molecular glue" that binds to metals, such as those in the catalytic molecules. The ligands also show an affinity for the surface of ceramic

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substrates, and thus promote the deposition of the molecules in a thin layer on the substrate.

Depositing the single layer of molecules is more difficult, albeit more efficient, than creating the more common multiple layers. Molecules on all but the top of multiple layers are ineffective, and thus are wasted in catalytic reactions, White said. But other, more subtle benefits of the single layer exist, as well.

"By forming a single layer you can effect a great deal of control on the structure that these special molecules will form on the ceramic oxide surface," he said. "You must know the structure to relate it to properties."

The researchers developed a family of copper-containing catalysts, each of which includes the exact same amount of copper -- between one and two percent by weight. However, the initial arrangement of the copper atoms varies systematically in each catalyst. One, for example, contains single copper atoms separated from each other by about five angstroms. Another catalyst contains pairs of copper atoms, a third contains triplets, and a fourth contains groups of six copper atoms. The ensembles of atoms in each catalyst are about five angstroms apart. Researchers verified the structures of the substances using selective chemisorption, electron paramagnetic resonance and transmission electron microscopy.

The researchers then incorporated the catalysts into

several important industrial reactions and studied the results. The addition of hydrogen to acetaldehyde proceeded with all four catalysts present, but the distribution of the products that resulted from each catalyst were different. Only the catalysts having two or more copper atoms per ensemble were active in the decomposition of methanol; the catalysts having six atoms per ensemble were active in the synthesis of methanol and ethanol from methyl acetate and hydrogen, White said.

"We chose these types of reactions because we expected that they would have vivid results -- yes/no types of answers," he said. "Our contribution is bringing a little more certainly to understanding and explaining the results of catalytic action. We offer the ability to produce good catalysts without much trial and error or empiricism."

The processes the researchers have studied could be applied to the making of fine chemicals, substances that are expensive to create and are used in small amounts in products such as detergents. The catalysts the researchers have developed would be useful in such processes because they could provide high quality control and selectivity, White said.

The technology could also be used in creating chemical barriers for protective clothing that would adsorb harmful chemicals, such as nerve gases, blistering agents, toxic wastes, and lethal fumes

produced during fires.

In other applications of this work, White and Dr. Mark Mitchell of Clark Atlanta University's Chemistry Department are trying to determine for the U.S. Department of Energy the optimum structure of a catalyst that could remove sulfur dioxide and nitrogen oxide from power plant flue gases.

White is also studying the reduction of methyl acetylene into propylene -- the starting material for plastic. The current way of doing this creates a lot of a high molecular weight side product, and a tendency for any propylene created to be turned into propane. White and his colleagues are finding that a catalyst they've made converts methyl acetylene to propylene with no propane formation, and very little of the high molecular weight side product.

The catalyst research is funded by Georgia Tech's Focused Research Program in Surface Science and Catalysis, which is directed by White and Dr. J.A. Bertrand, School of Chemistry.

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