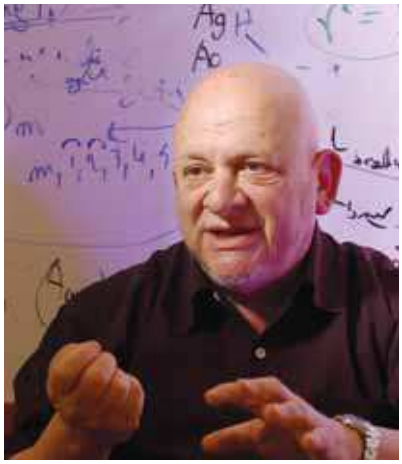
Charging nanocatalysts to reduce costs

Studying nano-sized clusters of gold on a magnesium-oxide surface, researchers at the **Georgia Institute of Technology** and **Technical University Munich** have found evidence for the electrical charging of nano-sized catalysts. The findings may prove to be an important factor in increasing the rate of chemical reactions during the manufacture of a range of materials from plastics to fertilizers.

"The fabrication of most synthetic materials involves using catalysts to promote reaction rates," said Uzi Landman, Director of the Center for Computational Materials Science, Regents' Professor, and Callaway Chair of Physics at Georgia Tech. "Designing catalysts that are more efficient, more selective, and more specific to a certain type of reaction can lead to significant savings in manufacturing expenses. Understanding the principles that govern nanocatalysis is key to developing more effective catalysts."

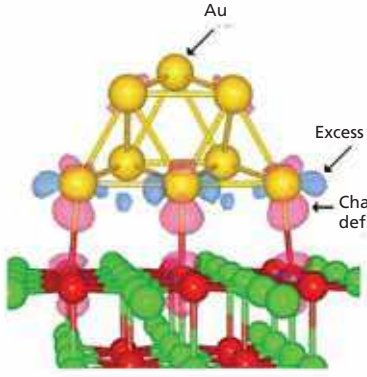
The study builds on joint research done since 1999 by the two groups that found gold, which is non-reactive in its bulk form, to be a very effective catalyst when it is in nanoclusters of eight to about 24 atoms in size. Those specific sizes allow the gold clusters to take on a 3-D structure, which is important for its reactivity.



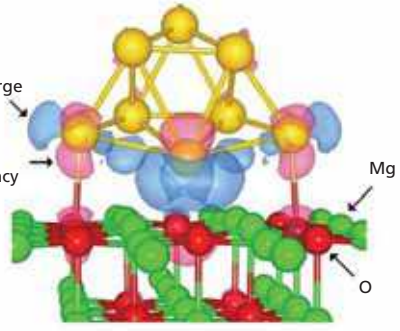
Georgia Tech professor Uzi Landman and colleagues are studying the particulars of nanocatalysis, which they believe will lead to the manufacturing of synthetic materials at lower costs.

"It is possible to tune the catalytic process not only by changing the composition of the materials, but also by changing the cluster's size, atom by atom," said Ueli Heiz, Professor of Chemistry at Technical University Munich.

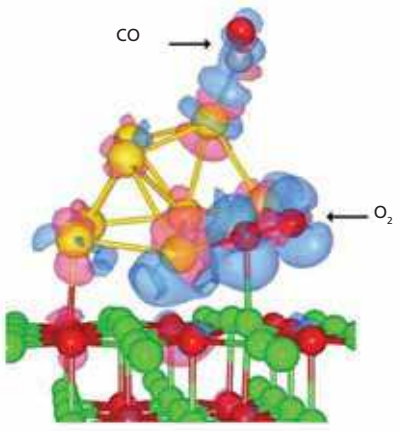
In earlier studies of the reaction where



Charge difference for a bare gold octamer supported on a perfect magnesia, (MgO) surface.



Charge difference for the cluster anchored on an oxygen-vacancy surface F-center, showing enhanced charging of the cluster.



Charge difference for the cluster with adsorbed reactants, supported on a surface F-center, showing charging of the CO and O_2 molecules.

carbon monoxide and molecular oxygen combine to form carbon dioxide, Landman's group used computer simulations to predict that when gold nanoclusters of eight atoms are used as the catalyst and magnesium oxide is used as the catalytic bed, reactions would occur when the bed had defects in the form of missing oxygen atoms, but would not occur when the magnesium oxide was defect-free.

Heiz's experiments confirmed this prediction, and the teams concluded that the gold must be anchoring itself to the defect where it picks up an electron, giving the gold a slight negative charge. Theoretical simulations showed that the electronic structure of the gold clusters match up with the oxygen and carbon monoxide. The charged gold transfers an electron to the reacting molecules, weakening the chemical bonds that keep them together. Once the bond is weak enough, it breaks, allowing reactions to occur.

Using eight-atom gold clusters as the catalyst and magnesium oxide as the catalytic bed in the most recent study, the team measured and calculated the strength of the bonds in the carbon monoxide by recording the frequency of the molecule's vibrations.

"If carbon monoxide is a strong bond, then there is a certain frequency to this vibration," said Landman. "If the bond of the carbon monoxide becomes weaker, then the frequency becomes lower. That's exactly what we saw—when we had defects in the magnesium oxide, we had larger shifts than when we had magnesium oxide without defects."

"And all this happens at low temperatures," said Heiz. Reactions requiring catalysts typically need heat or pressure to get the reaction going, adding to manufacturing costs. Since the properties of the catalytic beds can increase the rate of reactions for nanocatalysts, new and better low-temperature catalysts may be found.

"We knew the specific number of atoms in the catalyst and that defects in the catalytic beds are important. Now we know why those defects are so essential—because they allow the catalyst to be electrically charged," said Landman. "It's possible that at the nanoscale you may find catalysts that can do things under more gentle and cheaper conditions."

Jean L. Broge

Solutia nylon for mirror brackets

A nylon compound developed by **Solutia** is being used for exterior mirror brackets on the 2005 **Ford** Freestyle.

The material, Vydyne R543H, delivers the required performance while being more cost-effective than polyesters or magnesium, according to John Jurecko, Automotive Marketing Manager for Solutia's Vydyne nylon.

The Solutia Vydyne Automotive team worked with **Lear** and **Bing Assembly Systems** to develop and launch the

Briefs

In what they call the automotive industry's first global alliance for production of thermoplastic vulcanizate (TPV) sealing systems, **Jyco Sealing Technologies** and **Inoac** have formed a joint venture, **IJJ**. Jyco specializes in TPV sealing systems and will provide process technology and design services. Inoac will direct the manufacture of existing Jyco sealing systems in a new plant in Shanghai, China.

Demand in the United States for nanomaterials is expected to grow from $263 million in 2003 to $1.4 billion by 2008 and $34 billion by 2020—a 33% annual growth rate. This forecast comes from industrial market research company **Freedonia Group**, which says health care (mainly pharmaceuticals) and electronics will lead the way in nanomaterials demand. Prices are expected to drop as these markets are penetrated, leading to opportunities in automotive and other industries.

Mercedes-Benz will install non-leather interiors in all of its future models for customers who make such a request. The replacement of leather with another material will be done either at the factory or the dealership. It takes four cows to make one leather interior for a Mercedes-Benz, according to People for the Ethical Treatment of Animals.

Arcelor and **ThyssenKrupp Stahl** will combine research and development efforts in the area of highly resistant and highly formable flat carbon steels—specifically high-manganese steels—for automotive applications. Targeted is a 20% mass reduction in structural and chassis applications. The first new product is expected to be available by 2006.

Owens Corning and **RheTech** have reached an agreement under which the latter will manufacture and sell in North America a proprietary long-fiber glass/polyolefin thermoplastic developed by the former. The plastic has been available in North America only as an import; production will begin in the third quarter at a factory in Michigan.

Solutia worked with Lear and Bing Assembly Systems to develop the Ford Freestyle's exterior mirror brackets.

exterior mirror brackets for the Freestyle and the Ford 500, both of which went on sale in late 2004. The Vydyne team contributed to improving time-to-market by providing quick-response engineering support.

"The mirror bracket is one of the most critical components of the overall mirror design," Jurecko said. "The bracket must possess the optimal balance of stiffness, strength, and vibration damping in order to keep the mirror steady with the vehicle."

The company has been working on the mirror bracket applications for many years, according to Jurecko.

"We pay close attention to the latest trends in styling, such as larger mirrors for SUVs and heavy trucks located farther from the vehicle, and also understand the demands and challenges they pose such as managing increased drag," he said. "This places more demands on mirror brackets than ever. Mirror bracket designers need materials that have good strength-to-weight ratios, high stiffness, and frequency characteristics that address NVH requirements. Minimizing exterior mirror vibration is important to designers so they can improve the driver's view of his or her surroundings."

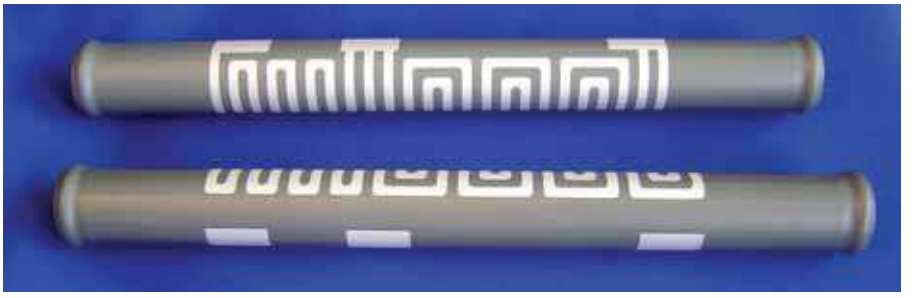
The Vydyne Automotive team used mold-flow analysis for the Ford mirror bracket, and it has begun development of mirror brackets for several other vehicles, Jurecko noted.

Solutia, in January, announced formation of the Vydyne Automotive global development team. The company has added personnel in North America, Europe, and Asia to support anticipated growth in applications of its nylon products. Vydyne nylon resins are used in a variety of automotive applications.

Patrick Ponticel

Putting the heat on

TT electronics IRC Wirewound & Film Technologies Division has developed a tubular aluminum substrate resistive technology that delivers tightly controlled "instant on" heat with greater than 95% efficiency, it claims. The technology provides OEM design engineers with a source of instant heat for cabin air, engine fluids, and other applications, such as for equipment that operates in extreme climates



IRC's Anotherm consists of rugged thick-film resistive elements deposited on tubular anodized aluminum substrate material for a number of applications, including "instant on" cabin heat for diesels, wiper fluid heaters, EGR air intake heaters, fuel pump flow controls, and more.

where oil pan heaters are required, or other engine fluids need to be protected from frigid temperatures.

The Anotherm Series devices consist of rugged thick-film resistive elements deposited on tubular anodized aluminum substrate material that can be tailored for "virtually any" heating application. The low thermal mass of the aluminum substrate provides "instant on" and "instant off" capabilities, and by using multiple "zones" of resistive circuitry, precise temperature control is possible.

"Today's diesel and hybrid vehicles do not produce sufficient engine heat to supply cabin air at the proper temperature, especially during the engine's warm-up period," said Wilson Hayworth, Product Manager at IRC's Wire and Film Division. "In addition to supplying heated cabin air, the lightweight Anotherm tubular heaters can be used to instantly boost defroster air temperature to eliminate window fogging in cold weather."

Hayworth added that for fluid applications, the Anotherm inline heaters provide systems engineers "significant design advantages, including a single-piece construction with integral hose fittings, unobstructed fluid flow, and precise temperature control. Our engineering team can develop custom circuitry to deliver the specific power density needed for each type of automotive fluid."

Anotherm's rugged thick-film resistive elements can also serve as voltage drop sources for systems such as daylight running lamps, HVAC fans, or radiator fan controls. When connected in series with these devices, the resulting voltage drop will provide slower fan speeds, dimmer lights, *etc.* The same Anotherm device can be used for multiple heating and voltage drop applications in the same vehicle.

Additional applications for the patent-pending Anotherm tubular heaters include diesel fuel warmers, wiper fluid heaters, EGR air intake heaters, heated seats and steering wheels, fuel pump flow controls, air brake purge valve heaters, rearview mirror deicing, and fuel cell heaters.

The Anotherm substrates are made from 6061 or 6063 aluminum alloy, with an insulation system consisting of a thin layer of anodized aluminum oxide chemically grown on the outer diameter of the aluminum tube, producing a dielectric layer approximately 0.0014 in (0.035 mm) thick, which provides an inorganic insulation that is not affected by temperature or chemical exposure.

This rugged construction gives Anotherm technology the ability to operate in extreme temperatures—up to 300˚C (572˚F) continuous operation. The Anotherm material can presently be made in diameters from 0.5 to 1.5 in (12.7 to 38 mm) outer diameter by 9 in (229 mm) in printed length.

Jean L. Broge