Scientists find evidence of electrical charging of nanocatalysts

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Researchers at the Georgia Institute of Technology and Technical University Munch have discovered evidence of a phenomenon that may lead to drastically lowering the cost of manufacturing of materials from plastics to fertilizers. Studying nano-sized clusters of gold on a magnesium oxide surface, scientists found **direct evidence for electrical charging of a nano-sized catalyst**. This is an important factor in increasing the rate of chemical reactions. The research will appear in the 21 January, 2005, issue of the journal Science, published by the AAAS, the science society, the world's largest general scientific organization.

"The fabrication of most synthetic materials that we use 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 current study builds on joint research done since 1999 by the two groups that found gold, which is non-reactive in its bulk form, is a very effective catalyst when it's in nanoclusters of eight to about two dozen atoms in size. Those specific sizes allow the gold clusters to take on a three-dimensional structure, which is important for its reactivity.

"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," explained Ueli Heiz, professor of chemistry at Technical University Munich.

In these earlier studies of the reaction where 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.

Now, in this latest study, the group has found direct evidence that this is indeed what is happening. Using eight-atom gold clusters as the catalyst and magnesium oxide as the catalytic bed, the team measured and calculated the strength of the bonds in the carbon monoxide by recording the frequency of the molecule's vibrations.

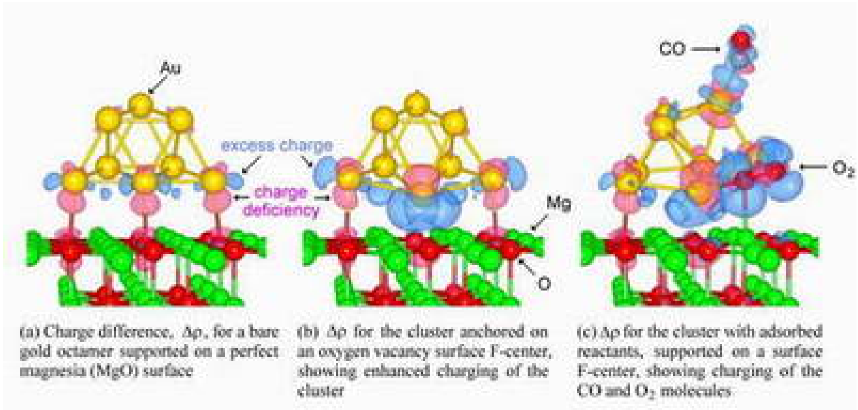

Diagram of charging.

"If carbon monoxide is a strong bond, then there is a certain frequency to this vibration," explained 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."

Lead author of the paper and senior research scientist in Landman's group Bokwon Yoon commented, "The agreement between the predicted and the measured values of the vibrational frequency shifts is very gratifying, confirming the charging and bonding mechanisms."

"And all this happens at low temperatures," said Heiz. Typically, reactions requiring catalysts need heat or pressure to get the reaction going, and that adds to the cost of manufacturing, but that isn't the case here. 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. We hope these guidelines will lead to more research in search of nano-sized catalysts. It's possible that at the nanoscale you may find catalysts that can do things under more gentle and cheaper conditions," said Landman.

Source: Georgia Institute of Technology

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