

## New Direction for Designing Catalysts for Automobile Exhaust Gas Purification Using Cuprates

Scientists of the "New Development of Novel Self-Forming Nanoparticle Catalyst without Precious Metals" research group have clarified the mechanism underlying the activity of a catalyst used to purify automobile exhaust gases and obtained a new direction for designing novel catalysts on the basis of their findings. This research is part of the Elements Science and Technology Project supported by the Ministry of Education, Culture, Sports, Science and Technology. The core organization in this project is Japan Atomic Energy Agency (Project Leader, Yasuo Nishihata), and the other participating organizations are Osaka University (Chief Scientist, Hideaki Kasai), Daihatsu Motor, Co., Ltd. (Chief Scientist, Hirohisa Tanaka), and Hokko Chemical Industry, Co., Ltd. (Chief Scientist, Senshu Mitachi). A press conference was held to announce the findings on (Tuesday) 7 February 2012.

Currently, precious metals such as rhodium (Rh), palladium (Pd), and platinum (Pt) are used as catalysts for the purification of automobile exhaust gases. The scientists of the research group theoretically analyzed the purification activity of catalysts containing transition metals and performed demonstrative experiments using the SPring-8 beamlines BL14B1, BL14B2, and BL28B2, with the aim of designing novel catalysts that do not contain rare precious metals. They evaluated the interaction between nitrogen monoxide (NO) and Rh, which is a precious metal exhibiting particularly high activity in the purification of NO contained in automobile exhaust gases, in addition to clarifying the differences between Rh and other precious metals and investigating the factors promoting the reduction of NO. From the results obtained, they found that Rh has a dissociative adsorption structure more stable than that of other precious metals, as well as a smaller activation barrier of dissociative adsorption, which allows NO to be easily separated.

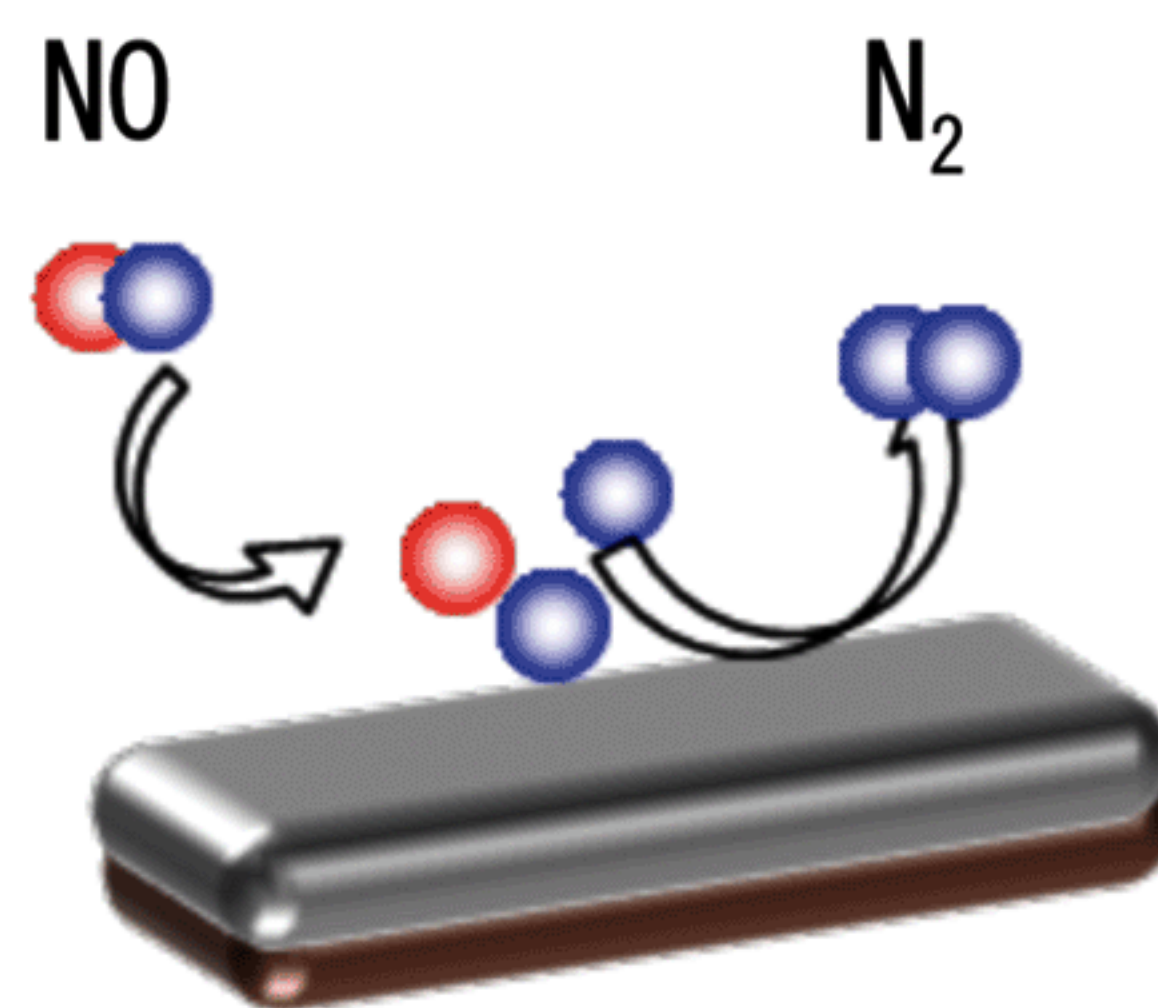
The scientists at Osaka University theoretically analyzed the dissociative adsorption of NO on the surfaces of various transition metals such as nickel (Ni), cobalt (Co), iron (Fe), and copper (Cu), and their oxides. The results revealed that

the surfaces of Ni, Co, and Fe were easily oxidized in the presence of oxygen (O) and that O atoms adsorbing onto the surfaces disturbed the dissociative adsorption of NO. On the other hand, the surface of Cu became more easily exposed than that of the other transition metals, and the purification activity of Cu was inferior to that of Rh even though NO was reduced on the exposed Cu surface. Moreover, the reason for the less active dissociative adsorption of NO by Cu was found to be due to the electron state of the Cu surface.

The scientists examined the electron state and catalytic activity of copper(I) oxide ( $\text{Cu}_2\text{O}$ ), a cuprate, to realize Cu with a similar electron state on its surface to that of Rh. They designed a structure that can be realized by oxidizing Cu then removing O atoms from the Cu surface and found that this structure promoted the dissociative adsorption of NO.

From the above theoretical findings, a new direction for designing novel catalysts for the purification of  $\text{NO}_x$  was obtained, which is expected to lead to the decreased use of precious metals. Significant advances in the practical application of new catalysts are also expected to be made on the basis of the findings. The results of this study were presented on 15 February at nano tech 2012, The 11th International Nanotechnology Exhibition and Conference, which is the world's largest fair of state-of-the-art nanotechnology.

(Related patents: 22 patents granted in Japan, 1 patent pending overseas)



Controlled surface of cuprate