# Moisture Changes Drastically the Catalysis of Gold Nanoparticles

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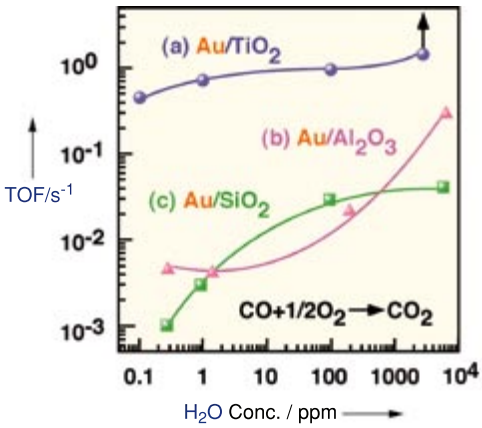
It was originally found in the late '80s in AIST that 'noble' gold exhibits high catalytic activities when its size is reduced to less than 5 nm. Among a variety of the reactions catalysed by gold nanoparticles, low-temperature CO oxidation has been most intensively studied. We have investigated moisture effect on this reaction for $Au/TiO_2$, $Au/Al_2O_3$ and $Au/SiO_2$ over a wide range of concentrations, ~0.1 to 6,000 ppm, and found that the activity is enhanced no less than two orders of magnitude. The effect of moisture strongly depends on the type of support oxide.




Reaction rates of CO oxidation (represented by turnover frequencies, number of CO molecules converted by a surface Au atom per second) over $Au/TiO_2$, $Au/Al_2O_3$ and $Au/SiO_2$ as a function of moisture concentration in the reactant gas.

# Mechanism of Peculiar Chemical Reactions in Supercritical Water Clarified

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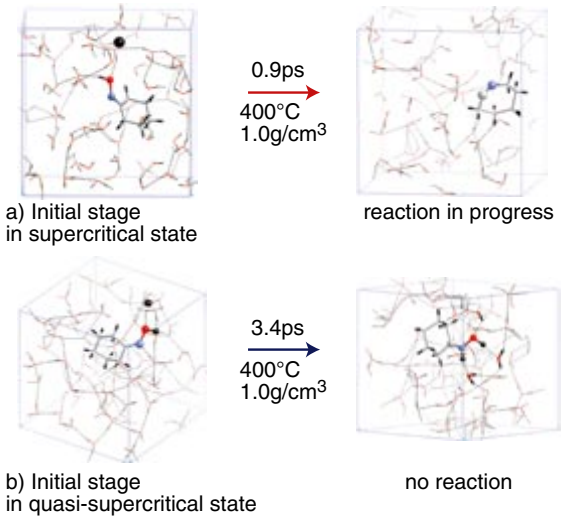
We have successfully opened the way to understanding the mechanism of peculiar reactions taking place in supercritical water. One of reactions in question refers to the Beckmann rearrangement where ε-caprolactam is produced from cyclohexanone oxime in supercritical water without using concentrated sulfuric acid, which was experimentally demonstrated by the SFRC-AIST. It has been successfully demonstrated, first in the world by the computer simulation based on the first principle molecular dynamics, that the rearrangement is made through incomplete hydrogen bond network created owing to peculiar density property of supercritical water, neither liquid nor gas, but an intermediate state between them.




Computer simulation of chemical reaction with a hydrogen ion added.