第340回触媒化学研究センターコロキウム

NO_x Storage Mechanism on NSR Catalysts

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2014年2月13日（木）15:00—17:00

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The need for fuel economy and consequently a reduction in CO_2 emissions for environmental protection has brought about the lean-burn engine technology with high air/fuel ratio for motor vehicles. However, the conventional three-way catalysts (TWC) in removing engine exhausts are no longer effective in reducing NO_x . The NO_x storage and reduction (NSR) method, first developed by Toyota researchers in 1995, is one of the leading strategies to tackle this issue. The catalyst works with alternatively lean and rich conditions: NO is oxidized to NO_2 on the precious metal, which is then stored in the form of nitrate on the BaO storage material under long fuel-lean conditions. Subsequently, the stored NO_x is reduced to N_2 under short fuel-rich conditions. As the storage process is of vital importance to the performance of the NSR catalyst, much attention has been focused on the deep understanding of the NO_x storage mechanism. Up to now, however, all theoretical works in the literature only focused on thermodynamics. No detailed mechanisms concerning the transition states and reaction barriers have ever been reported. In the present work, we will first study how site and size of$(BaO)_n$ clusters affect the NO_2 adsorption. With this understanding, we will further explore the detailed NO_2 reaction mechanisms by using an embedded cluster modeling.

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Professor Xin Xu received his Doctoral Degree in Theoretical Chemistry from Xiamen University, China, in 1991. After a postdoctoral stay at Fujian Institute of Research on the Structure of Matter, Academia Sinica, he was appointed as an associated professor in 1993 and was promoted to a full professor in 1995 in the department of chemistry, Xiamen University. He was also affiliated to the State Key Lab of Physical Chemistry on Solid Surfaces (PCOSS), China, where he acted as deputy director from 1996 to 2003. He was a visiting professor at Kyoto University, Japan, Ecole Normale Superieure de Lyon, France, and a visiting associate at California Institute of Technology, USA. From 2006, he was appointed as Lu-Jia-Xi Chair-professor of Xiamen University. From 2010, he moved to Fudan University, where he currently is the Chang-Jiang chair professor. His research interests involve development of density functionals and linear scaling quantum chemical methods, modeling of reaction mechanisms on the solid surfaces and in solutions.