**First-principles theoretical study of catalytic reactions at surfaces and interfaces**

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Chemical reactions at surfaces and interfaces play important roles in wide varieties of applications such as hegerogeneous catalysis, electrochemistry, fuel cells, batteries, etching processes of semiconductor materials, and so on. In this talk, we will present theoretical investigation and prediction of hydrogenation of CO2 over Cu catalyst[1]. Adsorption and reaction of CO2 on solid surfaces are attracting growing interest because of their importance in industrial, energy and environmental management. To clarify reaction mechanisms and to identify important factors governing the reactivity of CO2 on solid surfaces are very important to develop more efficient catalysts or catalytic processes for utilization of CO2. To this end, we investigated CO2 adsorption and hydrogenation[1] on Cu surfaces using van der Waals density functionals as implemented in our home made STATE (Simulation tool for Atom TEchnology) program code [2]. We theoretically proposed a new reaction scheme to enhance the hydrogenation of CO2 on Cu.

In the second topic, we will discuss enhancement of NO dissociation by hydrogen bonding. Nitric oxide (NO) emission from the exhaustive gas of combustion process has caused negative impacts on the environment, e.g, acid rain, photochemical smog, and ozone depletion. So far, catalytic activities for NO dissociation on the Cu surfaces have been recognized to be lower than that on Rh. Shiotari *et al*. experimentally found that the hydrogen bond between NO and water monomers promotes the NO dissociation to take place almost barrierlessly on the Cu(110) surface at a very low temperature (~12 K), which is a promising way to reduce the use of the precious Rh catalyst. would like to point out importance of the van der Waals density functional for describing . We present a DFT study to clarify the role of water molecules and the mechanism of the hydrogen bonding induced NO dissociation on the Cu(110) surface[3].

References

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