

# Analysis on the Catalytic Activity Improvement of Cu by Nano-Catalyst --Taking Ag and Cu Alloying as an Example

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**ABSTRACT:** In real life, nanotechnology has a wide range of uses, nanoparticles have large specific surface area, high activity, special foreign matter, small characteristics. Nanoparticles as catalysts is one aspect of the performance of nanomaterials. In this paper, taking Ag and Cu alloys as examples, the mechanism of nanocatalyzer is introduced, which significantly improves the catalytic activity of Cu, and the experimental application of converting mixed CO<sub>2</sub>/CO/H<sub>2</sub> materials into methanol (CO<sub>2</sub>+3H<sub>2</sub> → CH<sub>3</sub>OH+H<sub>2</sub>O) in industry is analyzed. In order to further optimize the activity of the catalyst, carbon nanotubes were introduced as the catalyst carrier, and single metal or alloy nanoparticles were loaded on the surface of the catalyst. Compared with the unsupported catalyst with the same alloy ratio, the catalytic activity of the prepared carbon nanotubes supported alloy nanocatalyst was significantly improved. Meanwhile, nanocatalysts have important applications in energy saving and environment protecting.

## 1. INTRODUCTION

Compared with ordinary catalysts, nanocatalysts have the essential conditions to act as catalysts. Due to the combination of the tiny size of the nanoparticles, the larger the percentage size of the sample on the surface, the different bonding and electronic states on the surface compared to the interior of the particles, and the incomplete coordination of the surface atoms leading to an increase in the active sites on the surface.

### 1.1. Nanomaterials

Nanoparticles are good catalysts due to their small size, the large volumetric fraction of the sample on the surface, the different chemical bonding and electronic states on the surface compared to the interior of the particle, and the incomplete atomic coordination on the surface, leading to an increase in the active sites on the surface, thus providing the basic conditions to act as catalysts. According to studies, when the particle diameter is lowered from 10nm to 1nm, the number of atoms on the surface increases from 20% to 90%. This not only results in a severe shortage of surface atom coordination, the formation of unsaturated bonds, and an increase in surface defects, but it also results in an increase in surface tension, which reduces the stability of surface atoms and causes them to seamlessly combine with other atoms to minimize tension.

## 2. APPLICATION

### 2.1. Catalysts in the chemical industry

Within the setting of renewable vitality capacity, the hydrogenation of carbon dioxide to methanol is vital in chemical fabricating. Utilizing thickness flooding hypothesis recreations, we explored the impact of copper cluster measure on the combination quality of both the reactants and the response intermediates, as well as the obstacles to actuating the fundamental response steps of carbon dioxide [1]. All of the fundamental response obstructions are directly corresponding to the adsorption energy of CO and O. We anticipate the medium-sized Cu<sub>19</sub> agglomerates to have the finest CO<sub>2</sub> hydrogenation reactivity in microkinetic recreations, likely due to the medium CO<sub>2</sub> overburden and decreased CO<sub>2</sub> delocalisation impedance. The catalytic execution is closely related to the electronic composition of the actuation location, which depends primarily on the estimate and neighborhood surface topology of the metal clusters or nanoparticles. Wang et al. used density functional theory (DFT) calculations to investigate the interaction of carbon dioxide molecules with the Cu (HKL) surface. The adsorption energy of periodic plates is lower when compared to experimental and cluster model data [2].

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## 2.2. Analytic technique

### 2.2.1. DFT count

The spin-polarised DFT calculations use a projector-enhanced wave (PAW) potential and a Perdew-Burke-Enzehev (PBE) function. The p (11) plate model used here contains a layer of copper atoms with a thickness of at least 20a separated by a vacuum of 15a to determine the exact surface energy. At a force convergence threshold of 0.02 e V/A, all atoms in the plate are completely relaxed. The interface force is determined from  $E_{sur} = (E_{slab} - NE_{bulk})/2A$ , where  $E_{slab}$  and  $E_{bulk}$  are the total energy of the plate and one volume of Cu atoms respectively, N is the number of Cu atoms in the plate and A is the surface

area. the structure of the Cu<sub>79</sub> cluster is determined from the calculated surface energy.

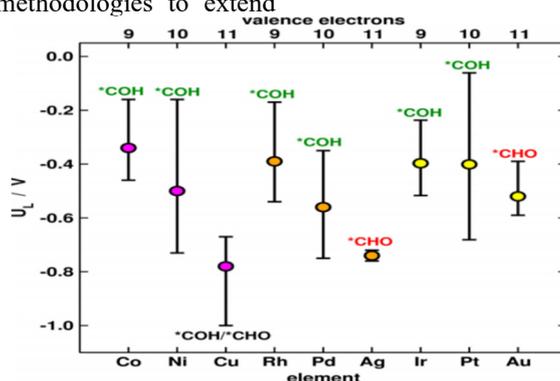
Chemisorption and activation of carbon dioxide on village clusters (n=7, 13 and 19) have been shown to be effective [8]. The positive adsorption energy of carbon dioxide on the village cluster indicates that the adsorption process has thermodynamic advantages. The researchers found that carbon dioxide molecules adsorb on one of the vertices of the icosahedral Cu<sub>13</sub> cluster and, as a precursor, have the largest adsorption energy (52.47 kcal.mol<sup>-1</sup>). Preferentially adsorbed sites for carbon dioxide molecules have been identified. In NPA analysis, the interaction between Cu clusters and CO<sub>2</sub> molecules leading to CO<sub>2</sub> speciation has been understood by charge transfer in NPA analysis.

**Table 1.** The most stable adsorbent formed during the first hydrogenation of CO

Metal	111 cn=9	100 cn=8	211 cn=7	211k cn=6	3AD@111 cn=5
Co	*COH	*COH	*COH	*COH	*CHO
Rh	*COH	*COH	*COH	*COH	*COH
Ir	*COH	*COH	*COH	both	*COH
Ni	*COH	*COH	*COH	*COH	both
Pd	*COH	*COH	*COH	*COH	*COH
Pt	*COH	*COH	*COH	*COH	both
Cu	both	both	*CHO	*CHO	*CHO
Ag	*CHO	*CHO	*CHO	*CHO	*CHO
Au	*CHO	*CHO	*CHO	*CHO	*CHO

As appeared in Table 1, specialists accept that the foremost abundant response middle of the road in \*CO hydride responses is by and large \*COH, and that Cu, Ag and Au tend to make \*CHO [5]. In expansion, for of a few metals, as with Cu, Ag and Co, \*COH and \*CHO coexist, which depends on the number of ligands within the activity location. Since \*CHO and \*COH tie to substrates in an unexpected way, plan methodologies to extend

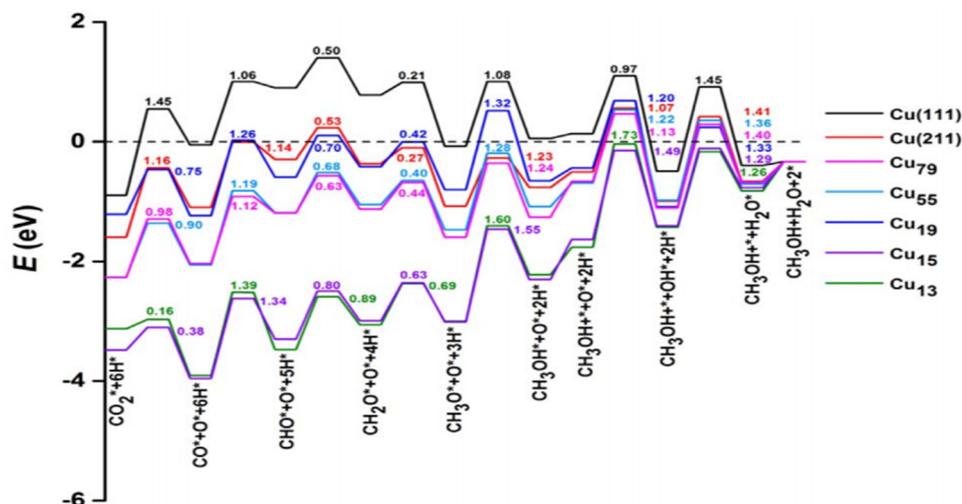
catalytic movement by modifying \*CHO authoritative can as it were sometimes modify \*COH incorporation. Figure 1 demonstrates the beginning potential (famous as UL) is checked as the move control or idle constrain of the basic restriction organize, in this particular case  $*CO + H^+ + e^- \rightarrow *CHO$  or  $*CO + H^+ + e^- \rightarrow *COH$  [3].



**Figure 1.** Electrochemical potentials required for the CO hydrogenation

Figure 2. clearly shows that the higher the current obstructions for hydroxylation of CH<sub>n</sub>O bound, the more grounded the adsorption on CH<sub>n</sub>O (n=0-3) intermediates and H molecules. The auxiliary affectability of CH<sub>n</sub>O (n=0-3) is regularly lower than that of CO<sub>2</sub> breakdown [8]. The creation of HCO intermediates incorporates a gigantic

boundary within the run of 1.06-1.39eV, but acetaldehyde and CH<sub>3</sub>O generation is less difficult within the ranges of 0.50-0.09eV and 0.21-0.69eV, separately [7]. The obstruction to methanol generation from CH<sub>3</sub>O is the most prominent (1.08-1.60eV) [6, 7].



**Figure 2.** Carbon dioxide in copper clusters and extended surfaces at reduction potential surfaces. All basic reaction barriers are expressed in eV.

As can be seen from the DFT calculations, the reduction of carbon dioxide to methanol is very sensitive in terms of texture. The attraction capacity of all reagents, intermediates and products is linearly proportional to the adsorption energy of CO and O. Hence, the barriers to the positive and negative processes of the decomposition of the reaction associated with the reduction of CO<sub>2</sub> can be related to the attraction capacity of CO as well as O, which can be used as the main descriptor of the hydrogenation activity of CO<sub>2</sub> over copper catalysts. It can be seen that the more powerful the attraction energy of CO and O, the less the potential obstacles for CO<sub>2</sub> decomposition and the more the potential obstacles for the combined reaction of CO and O.

### 2.3. Nanocatalyst and environmental protection

Application of nanocatalyst in environmental protection. Automobile exhaust treatment CO. And NO gas are the main pollutants in automobile exhaust emissions. The supported NCs can effectively solve the problem of the mismatch between the temperature range of the catalyst and the temperature range of automobile exhaust gas, and the catalytic CO conversion rate can be as high as 83%. Experts confirmed by simulation experiments that in the presence of oxygen, PD-RHNCs showed a very high activity in the process of CO oxidation, and in the absence of oxygen, Pt-rhncs activity was higher; for NO reduction, pT-RHNCs showed high catalytic activity regardless of the presence or absence of oxygen [4]. In addition, Khoudiakov's research results show that the Au nanoparticles deposited on the transition metal oxide FeO also have high catalytic activity for CO oxidation at room temperature.

## 3. OTHER AREAS OF APPLICATION

### 3.1. nano-zeolite

Nano-zeolite has a high selectivity of catalytic activity due to their high adsorption capacity, tiny grain size, large specific surface area, and more active c-enters exposed on the outer surface. In the energy industry, nano-catalysts are used to achieve high hydrogen generation efficiency. The hydrogen generated can be utilized to power fuel cells. The conversion of carbon dioxide to methane is critical in the activation of methane. Increase the longevity, stability, and efficiency of fuel cells. To increase the synthesis yield, a nano-catalyst was added to the heterogeneous catalytic system. The use of nano-catalysts in industrial production benefits reactor efficiency, product structure modification, and effective yield growth. The industrial manufacturing method of isopropyl benzene (using ananomolecular sieve as a catalyst) may effectively address the corrosion problem, increase the yield of the target product, and decrease waste.

## 4. CONCLUSION

In summary, this paper introduces the characteristics and applications of nanocatalysts in the field of chemical industry, nano-catalysts improve the hydrogenation efficiency. As a good catalyst carrier, nanomaterials play an important role in the process of CO<sub>2</sub> transformation, which improves its conversion rate and reduces the cost of industrial production. In addition, the methanol produced is a good industrial fuel. The Cu-Ag alloy mainly introduced in this paper has good adsorption due to its special dodecahedron structure, and effectively uses the nano catalytic carrier to enhance the catalytic performance. Compared with the unsupported catalyst with the same alloy ratio, the catalytic activity of the prepared carbon nanotubes supported alloy nanocatalyst was significantly

improved. Meanwhile, nanocatalysts have important applications in energy saving and environment protecting.

## AUTHORS' CONTRIBUTIONS

This paper is independently completed by Heyang Xiu.

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