Iridium Surface Treatment by Glow Plasma Treatment and Its Application as Electrocatalyst for Methanol and CO Oxidation

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The regulation of the electrocatalytic activity of an iridium surface using a plasma activation treatment process has been studied experimentally and using first-principles calculations. The microstructures and catalytic properties were investigated using scanning electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy, cyclic voltammetry and CO-stripping voltammograms. The results show that the plasma activation treatment process can promote the surface energy of iridium particles, thereby increasing their surface activity as a catalyst. Furthermore, the current density of Ir/C-Plasma is 1.46 times higher than that of Ir/C, indicating that the electrocatalytic activity is significantly increased upon increasing the number of surface-active sites. More importantly, the mechanism of the surface activity sites that improves the catalyst performance of the iridium surface was illustrated using first-principle calculations. We also find that CH₃OH molecules form chemical bonds with the dangling bonds localized on the iridium atoms around the vacancies and that these sites have the lowest adsorption energy (−0.578 eV). Meanwhile, the TS results indicate that the dissociation of CH₃OH on a non-vacancy surface was more difficult than on the one-vacancy surface. In addition, the charge transfer further confirms that the vacancies on the iridium surface can provide a large number of active sites for chemical adsorption/desorption, which can promote CO anti-poisoning processes. This study not only reveals the CH₃OH adsorption/desorption reaction mechanism of Ir/C-Plasma, but also provides effective guidance toward improving the catalyst performance of noble metal catalysts.

Keywords: Electrocatalytic activity, iridium surface, first-principles calculations.

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