1P20 Quantum Chemical Study on the Precious Metal Electrocatalysts and Their Reactivity

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【Introduction】

In order to design more efficient electrocatalyst for the polymer electrolyte fuel cell, it is important to investigate the electrochemical processes at the electrode/electrolyte interface on both atomic and electronic levels. Recently we reported successful development of an accelerated quantum chemical molecular dynamics program "Colors", which is based on our original tight-binding theory. Thus, it enables us to simulate the chemical reaction dynamics for large systems considering the electronic states. In the present research, we investigated the electronic properties of Pt catalyst systems calculated by our accelerated quantum chemical molecular dynamics program.

【Computational methods】

The accelerated quantum chemical molecular dynamics calculations were carried out using the "Colors" program developed in our laboratory. This program is over 5,000 times faster than the conventional first-principles molecular dynamics approach.

【Results and Discussion】

We studied the graphite supported Pt_{13} particle by the "Colors" program. The Pt_{13} particle on graphite(001) surface (shown in Fig. 1) showed more complex charge distribution, due to the particle properties of Pt and effects from the graphite support. This graphite supported Pt_{13} particle shows positive charge in the vicinity of graphite(001) surface, while it shows negative charge at the surface that is far from graphite support. Based on the adsorption structure and the analysis of electronic state, the overlap of Pt-d orbital with p orbital of carbon on the graphite surface was observed(Fig.2). However, in the case of graphite(001) surface, this kind of overlap is very minor and therefore the interaction between Pt_{13} cluster and the graphite(001) surface is weak. This indicates that it is easy for the Pt_{13} cluster on the graphite(001) surface to sinter. The details of electrode reaction assisted by platinum catalyst will also be reported.

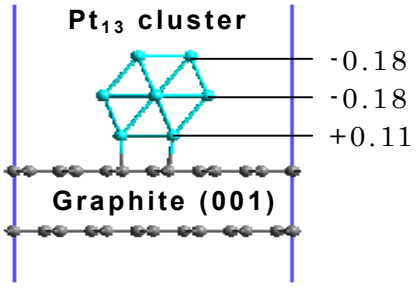

Fig. 1 The Pt_{13} particle on the graphite(001) surface.

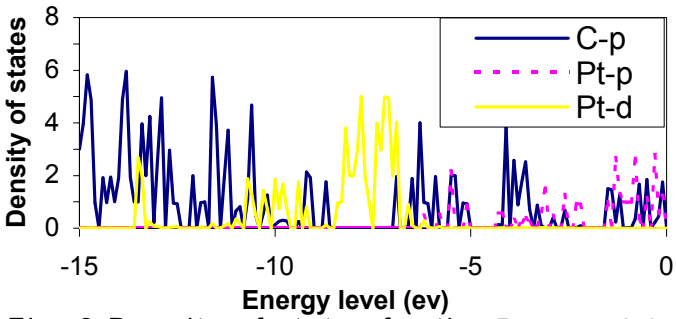

Fig. 2 Density of states for the Pt_{13} particle on graphite(001) surface.