

## Theoretical Study on the Electrical Conductivity and Electrocatalyst Reaction Properties of Polymer Electrolyte Fuel Cell Electrode

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### 【Introduction】

Polymer Electrolyte Fuel Cell (PEFC) has the advantage of high efficiency, high energy density and zero or low pollutant emissions. A PEFC consists of an anode where hydrogen is oxidized, a cathode where oxygen reduction occurs, and an electrolyte membrane that permits the flow of protons from anode to cathode. There are several challenging issues for PEFC commercialization. These include energy loss due to large overpotential and high material cost associated with high Pt loading and short lifetime of electrodes and electrolyte. The major cause of overpotential comes from oxygen reduction at cathode. In the present study, we focus on the electronic properties of oxygen reduction reaction (ORR) on the platinum catalyst systems by using our tight-binding quantum chemical molecular dynamics program New-Colors program.

### 【Method】

Tight-binding quantum chemical molecular dynamics and electrical conductivity calculations were carried out using New-Colors program developed in our laboratory. It realizes over 5,000 times acceleration compared to the conventional first-principles molecular dynamics method.

### 【Results and Discussion】

Carbon supported platinum (Pt/C) is the best-known electrocatalyst for both hydrogen oxidation and oxygen reduction in PEFC. We focused our attention to examine the ORR on Pt/carbon system. In order to approach more closely the real Pt electrode reaction, a complex model of one Pt<sub>4</sub> clusters on graphite(11-20) surface with nine water molecules, oxygen molecule, one hydronium ions and one CF<sub>3</sub>SO<sub>3</sub><sup>-</sup> was prepared as shown in Fig. 1a. From the simulation results, we observed that hydronium ion dissociated to water and proton, and then proton moved to the oxygen molecule. The new OOH group was formed (Fig.1b), after proton transfer to oxygen. Then, it is found that OOH decomposes into atop oxygen and hydroxyl adsorbed species on the Pt<sub>4</sub> cluster/graphite(11-20) system (Fig.1c). We discovered that the first proton transfer intermediate(OOH) was formed rapidly, similar to results reported by other DFT investigation[1,2]. On the other hand, we also investigated the ORR on Pt<sub>4</sub> cluster/different supported carbon (graphite(0001) and carbon nanotube) system. As we know, the electron transfer is important "KEY" during the oxygen reduction reaction (ORR). Therefore, it is necessary to study the electrical conductivity of the oxygen on the Pt/carbon electrodes. We constructed the 14 kinds of models of oxygen adsorption on Pt<sub>4</sub>/graphite(0001) by employing different O<sub>2</sub>-Pt<sub>4</sub>(from 1.2Å to 5.4Å)distance. The electrical conductivity of all the models was calculated by using our New-colors program. The model with 1.8Å (O<sub>2</sub>-Pt<sub>4</sub> distance) showed the highest electrical conductivity. Moreover, the electrical conductivity of O<sub>2</sub> on Pt<sub>4</sub>/different carbon (graphite (11-20) and carbon nanotube) system will be presented in the conference.

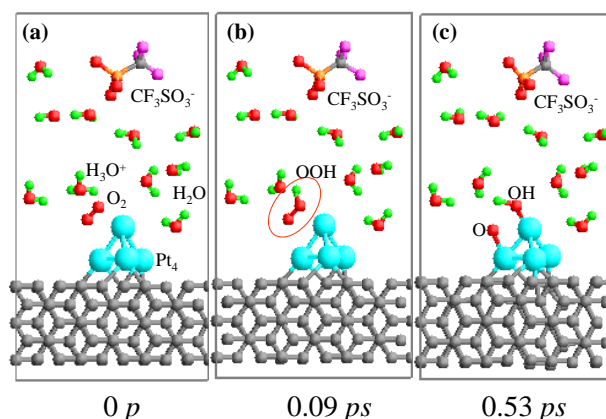


Figure 1 Complex model of Pt<sub>4</sub> supported by graphite(11-20) surface: (a) initial structure; (b)OOH intermediate formation; (c) OOH dissociation.

### References

- [1]Y. Wang and P. B. Balbunena, *J. Phys. Chem. B*, **109**, 14896 (2005).  
 [2]T. Li and P. B. Balbunena, *Chem. Phys. Lett*, **367**, 439 (2003).