INVESTIGATION ON STRUCTURAL AND ENERGETIC PROPERTIES OF CHITOSAN MEMBRANE SURFACE OF PEM FUEL CELL BY QUANTUM CHEMICAL CALCULATION

INTRODUCTION

At present, energy consumption continuously increases but many energy resources have decreased. Many researchers, now, try to find new ways to handle this problem. Fuel cell is one of them because of its advantages such as it is the environmental friendly electric power sources. Fuel cells works in the same way as conventional batteries, but have the major advantage that they do not run down over time and will go on producing electricity as long as this fuel supply does not run out. Using reformer technology, fuel cell can use hydrogen from hydrocarbon fuel, for example natural gas, methanol or even water.

Fuel cells have many types depending on their operations. Proton exchange membrane (PEM) is one of them. PEM fuel cell operates at low temperature, about 70-80 ^{o}C. So, this can drive them a prime candidate for powering the next generation of electric vehicles, and their modular design and the prospects of micro-scaling them have gained the attention of cell phone and laptop manufactures. The basic structure and operation principle the PEM fuel cell are illustrated in Figure 1. The PEM fuel cell is mainly constructed by a polymer such a Nafion as a membrane. The polymer electrolyte consists of a perfluorinated polymer backbone with sulfonic acid side chains. When fully humidified, this material becomes an excellent protonic conductor. The membrane and the two electrodes (teflonated porous carbon or cloth with platinum on supported carbon) are assembled into a sandwich structure to form a membrane electrode assembly (MEA). The MEA is placed between two graphite bipolar plates with machined that provide flow channels for disturbing the fuel (hydrogen) and oxidant (oxygen from air). The hydrogen rich fuel is fed to the anode, where the hydrogen diffuses through the porous gas diffusion electrode (GDE). At the catalyst layer, the hydrogen splits into hydrogen proton and electrons according to:

$$2H_2 \longrightarrow 4H^+ + 4e^- \quad (1)$$

Driven by an electric field, the H^+ ions migrate through the polymer electrolyte membrane. The oxygen in the cathode gas stream diffuses through the gas diffusion electrode towards the catalyst interface where it combines with the hydrogen protons and the electrons to form water according to:

$$O_2 + 4H^+ + 4e^- \longrightarrow 2H_2O \quad (2)$$

The overall reaction is exothermic and can be written as:

$$2H_2 + O_2 \longrightarrow 2H_2O + \text{electricity} + \text{heat} \quad (3)$$

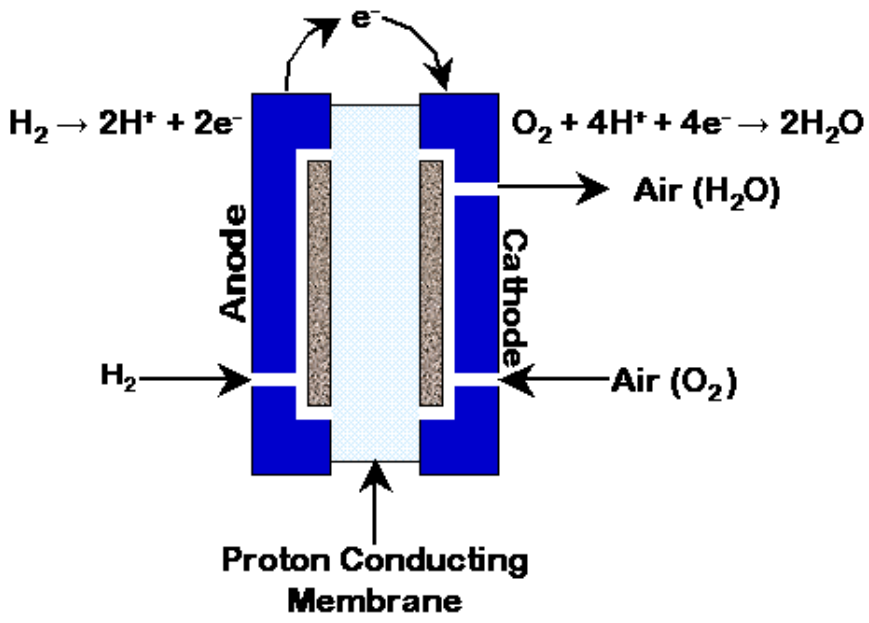

Figure 1 Schematic of PEM Fuel Cell

Source: www.lynntech.com/licensing/pem_fuelcell/index.shtml

The membrane of PEM fuel cell is originally made from polymer such as Naifon. So, there are many researchers have concerned with the polymer membrane and tried to find the best membrane giving the best performance of the cell.

Chitosan is one of the interesting membranes. Chitosan (pronounced kite-o-san) is a natural product derived from Chitin as shown in Figure 2, a polysaccharide found in the exoskeleton of shellfish like shrimp or crabs. It is not digestible but may have beneficial effects on the gastrointestinal tract It appears to reduce the absorption of bile acids or cholesterol; either of these effects may cause a lowering of blood cholesterol, however studies regarding its ability to lower cholesterol have been mixed. While it has been in existence for millennia, its current form has just recently been reported. Technically speaking, Chitosan is a naturally occurring substance that is chemically similar to cellulose, which is a plant fiber. Since Chitosan's structure is such polymer structure, some researchers have studied to possibility of making chitosan as the membrane for PEM fuel cell.

Because the PEM fuel cell has the polmer membrane and two electrodes, many researchers have focused on their structure and performance. Molecular modeling is such a way to determine their structure and also their transport mechanism during the operation. These in silico techniques have many advantages. For example, they eliminate the need of use real chemicals that is called greener science. Transport phenomena that would have been difficult to study experimentally can be studied with the virtual ease in silico, with mechanistic and chemical insights obtained.

The widespread availability and use of personal computer has resulted in molecular modeling and simulation techniques becoming a common research tools. Computational techniques are being used to study the science behind fuel cells, helping researchers to better understanding processes and experiment with the new approaches. Molecular modeling and simulation has been used to study new electrolyte material and surface catalysis for fuel cells.

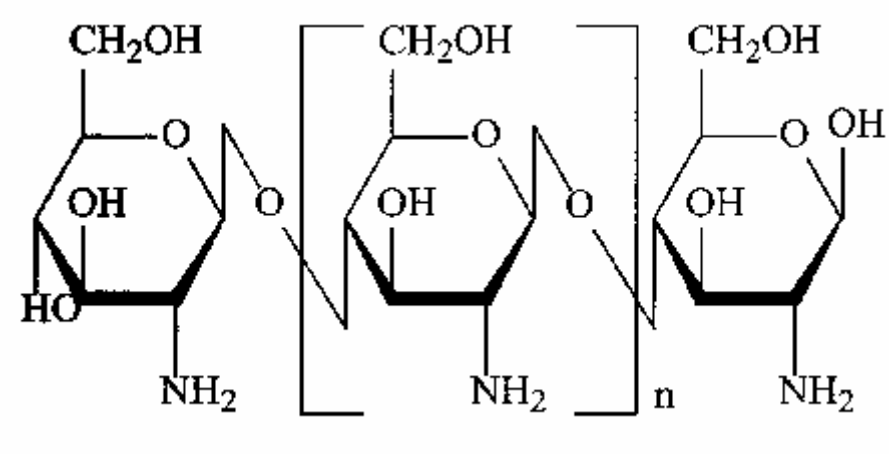

Figure2 Molecular Structure of Chitosan

Source: www.dalwoo.com/**chitosan**/**structure**.htm

Objective

To study and simulate structural and energetic properties of Chitosan membrane for PEM fuel cell by quantum chemical calculations.

Scope

This research is to study proton transfer mechanism in the membrane. The simulator named GaussW 03 and GaussView 3.0 will be the main tool for model, simulation and implementation.

Thesis Contributions

1. The molecular modeling and simulation can determine the mechanism and transport phenomena in PEM fuel cell for improvement of the cell.
2. The basic for design and production of PEM fuel cell manufactures