Vasavis Punnasukhirom 2006: Investigation on Structural and Energetic Properties of Chitosan Membrane Surface of PEM Fuel Cell by Quantum Chemical Calculations. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Associate Professor Thongchai Srinophakun, Ph.D. 68 pages.
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One of the factors influenced the performance of Proton Exchange Membrane Fuel Cell (PEMFC) is the ability of proton transfer in the membrane. The cell membrane can be made from biopolymer such as chitosan. In this study, the proton transfer in water environment mechanism throughout the chitosan membrane was investigated to enhance the performance of the cell. Molecular Modeling technique was used to determine the geometrical parameters of chitosan oligomers by semiempirical PM3, AM1, *ab initio* HF/3-21G* and HF/6-31G* based on Gaussian software. The results show that the geometrical parameters of chitosan oligomers, bond lengths; and bond angles are in the same range. In addition, the results were also compared with the parameters from X-ray crystallographical data with a good agreement. The electronic property of conducting polymer can be calculated by HOMO-LUMO method. In this study, the energy gap of chitosan polymer obtained from PM3 is 0.42 eV and 0.89 eV from HF/6-31G*. From these results, the chitosan polymer can be applied as the conducting polymer because of its near zero energy gap. The proton transfer by hopping mechanism was investigated with 3 water contents; 10, 35, and 90%. The optimum water content was found at 30% with the chitosan pentamer of 20 active sites. The number of electron from this oligomer is 20 and the electrical current is $3.2 \times 10^{-4}$ mA.

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