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SIMULATION STUDY ON AQUEOUS SOLUTIONS OF BIO-MOLECULES USED IN BIOFUEL CELLS

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Recent years much attention has been paid to the biofuel cells, which are expected as the next generation portable, clean, and safe chemical batteries that can be used even in a human body. Glucose is one of the most promising energy resources of biomass component used in a biofuel cell, because it is most abundantly found monosaccharide in the field. Based on the recent report, the enzymatic fuel cell has achieved ten times the energy storage of lithium ion batteries. Meanwhile, in recent years the biodegradable polymers are frequently used in the broad area, especially in the medical treatment, e.g. surgical suture, cartilage support, and capsules carrying drugs to the affected part. Poly Lactic acid (L-acid) and Poly Glycolic acid (G-acid) are typical examples, which resolute to L-acid and G-acid in a human body, respectively. According to the recent literatures, the biofuel cells using L-acid and G-acid have been constructed, which are expected to work in a human body and/or on a human skin. In the cathode of biofuel cells, e.g. glucose is oxidized to produce gluconolactone, as:

$$C_2H_{12}O_6 \rightarrow C_6H_{10}O_6 + 2H+ + 2e-.$$

Therefore, the glucose aqueous solution in the cathode of the biofuel cell contains many constituents including buffer solute. There are many molecular dynamics (MD) studies on glucose, L-acid, and G-acid aqueous solution, however, few MD studies have treated multi-component bio-molecule aqueous solutions. Recent years, we have been engaged in many MD studies on multi-component aqueous solutions including carbon dioxide, nitrate, sulfate, and amino acid ion etc. In this study, as a serial work, we wish to perform a simulation study on bio-molecule aqueous solutions as a model of a cathode of biofuel cell. In the simulation study, firstly, the structure and atomic charges of the constituents of the solution, i.e. glucose etc., are optimized using Gaussian09 on the basis of the density functional theory (DFT). Vibrational modes of ions will be discussed based on the structure difference. The transport properties, and thermodynamic properties of the solution will be examined by MD. The dielectric properties of solutions in various concentration of solutes will also be discussed.

Recent Publications

1. S Matsunaga (2017) Molecular dynamics study on carbon dioxide absorbed potassium glycinate aqueous solution. Journal of Solution Chemistry. 46(12):2268-2280.
2. S Matsunaga (2018) Structure and transport properties of AgI-AgCl-CsCl glasses: molecular dynamics study. Ionics. 24(5):1371-1376.
3. S Matsunaga (2017) Effect of sulfate anion on the structure and transport properties of seawater: A molecular simulation study. Journal of Molecular Liquids. 226:90-95.
4. S Matsunaga (2015) Effect of greenhouse gases dissolved in seawater. International Journal of Molecular Sciences. 17(1):45.
5. S Mastunaga (2014) Anomalous electrical properties in superionic (AgxCu1-x)Br (x=0.5): ab initio study. Ionics. 21(1):161-166.

Biography

Shigeki Matsunaga pursued his Master's Degree from Graduate School, Division of Natural Science, Niigata University in 1983; PhD Degree on the experimental and theoretical studies on compound forming liquid alloys at the same university; graduated from the Faculty of Science, Saitama University in 1981. He is a Professor of Physics at the National Institute of Technology, Nagaoka College. He is a Member of The Physical Society of Japan, The Japanese Society for Neutron Science, The Molecular Simulation Society of Japan, The Japan Association of Solution Chemistry, and The Physics Education Society of Japan. He received Grant-in-Aid for Scientific Research (C) from The Japan Society for the Promotion of Science: Project Year: Apr 2015 - Mar 2019, Apr 2010 - Mar 2013, and Apr 2005 - Mar 2009. His research interests include: structure and transport properties of the aqueous solutions of bio-molecules mainly used in a biofuel cell. Many MD studies on the structure, transport properties, and electric properties of the multi-component solid electrolytes, molten salts, and liquid metal alloys have also been performed.

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