Structure and Transport Phenomena of Non-Aqueous Electrolyte in Al Ion Batteries -Study by Molecular Dynamics-

Shigeki Matsunaga
National Institute of Technology, Nagaoka College, Nagaoka, Japan
matsu@nagaoka-ct.ac.jp

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1. Introduction

Li-ion batteries are widely used as power sources for smart phones and batteries for electric vehicles. However, Li is unevenly distributed on the earth and there is a concern about stable supply. Therefore, development of a secondary battery using an alternative element is required. Secondary batteries using aluminum ions have various advantages such as not only abundant Al as a raw material but also higher safety than lithium ion batteries. For this reason, it is drawing attention as a next-generation secondary battery [1].

However, when water is used as an electrolytic solution, it is decomposed and hydrogen is generated. Therefore, various organic solvents have been studied as electrolytes, such as 1–ethyl–3–methylimidazolium chloride, i.e. [EMIm]Cl. There are many MD studies of molecular liquids, but to our knowledge, there are not many simulations assuming the electrolyte of ion batteries.

In recent years, we have systematically carried out MD studies of multicomponent aqueous solutions. [2-5]. In addition, we have conducted research on aqueous solutions of glycolic acid and lactic acid used in biofuel cells [6-8].

As a part of a series of solution research so far, this study will perform MD simulations of molecular liquids as electrolytes for Al-ion batteries. First, the shape and charge of the molecule used for MD of the electrolyte are determined by density functional theory (DFT) using Gaussian.

2. Molecule preparation by DFT and MD procedure

The EMIm cation is in advance optimized to determine the configurations and charges of atoms by Gaussian09 using the density functional theory (DFT) at the B3LYP/6-311++G(d,p) level of the theory.

In MD, the interactions between EMIm and solute, Al^{3+}, Cl^-, are expressed as, $V_{ij}(r) = A/r^n - B/r^6 + z_i z_j e^2/r$, n = 12 or 9. MD is performed with NTP constant condition, at 293K, 1 atm.

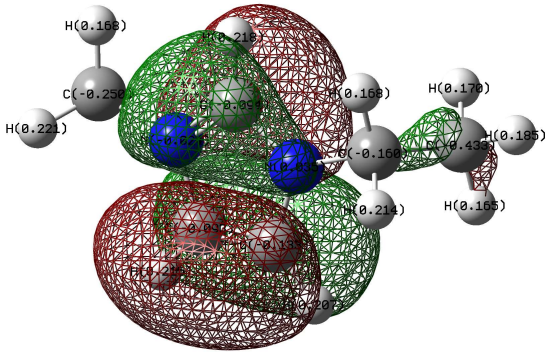

Fig 1. EMIm cation obtained by DFT.

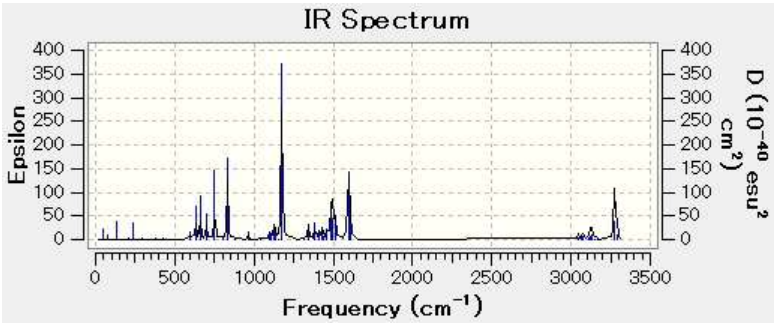

Fig 2. IR Spectrum of EMIm cation obtained by DFT.

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