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XAS measurements for ionic liquids: imidazolium salts

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1 Introduction

Ionic liquids have received much attention because of their versatile properties such as electrolytes in electrochemistry, environmentally friendly solvents in organic synthesis, and immobilizing phases for biphasic catalysis. They are also regarded as precursor materials for catalysts. Dialkylimidazolium and N-alkyl pyridinium or quaternary ammonium based salts are typical ionic liquids most widely studied due to the ease of synthesis. The completely ionic nature of ionic liquids makes them useful as solvents for highly charged complexes and the low vapor pressure of ionic liquids allows us to use them in vacuum and as "green" solvents in industrial processes. Moreover, when metal ion containing ionic liquids are prepared, a potential catalytic performance was observed. In this context, application of a new analysis technique on ionic liquids is awaited to clarify physical properties of ionic liquids.

XAS measurements for liquid samples have been enabled by Nagasaka, Kosugi and coworkers, giving new insights for physicochemical properties of materials [1]. In this project we have studied N-K edge XAS measurements for imidazolium salts to examine a possibility to find a novel aspect of ionic liquids by XAS measurements and analyses.

2 Experiment

XAS measurements for liquid samples were conducted at BL7A using facilities developed by Nagasaka et al. [1]. The liquid sample cell with SiC membranes was adopted, where the thickness of the liquid layer was controlled by the He gas pressure around the cell. The XAS spectra of the ProLINE polymer film were measured in parallel to calibrate the photon energies.

3 Results and Discussion

Fig. 1 shows N-K XAS spectra for 1-ethyl-3-methyl imidazolium chloride (EmimCl) 0.20 M and 0.10 M aqueous solution samples and 1-butyl-2,3-dimethyl-imidazolium chloride aqueous solution (0.10M). In all cases a sharp peak at 401.0 eV was found, indicating that this position is intrinsic to imidazolium N atom without dependence on concentration and substitute groups.

We also measured N-K XAS spectra for other related nitrogen-containing molecules (not shown). It was found that the peak position is dependent on the charge on nitrogen atom. For the simulation of the XAS spectra quantum chemical calculations and MD calculations including solvent molecules are underway. It is expected that measurements of N-K XAS would give the information on the charge of nitrogen atom.

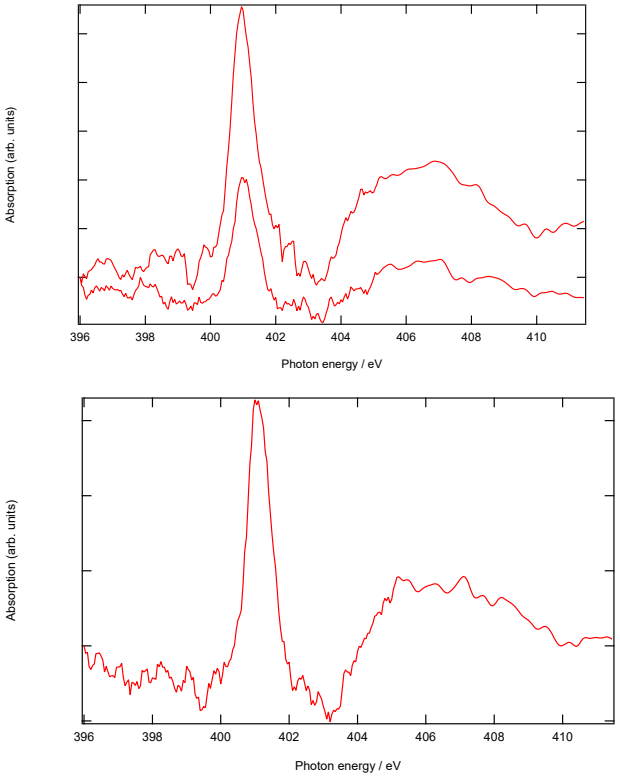

Fig. 1:N-K XAS spectra : Upper panel: EmimCl aqueous solution (Upper 0.20 M, Lower 0.10 M), Lower panel: 1-butyl-2,3-dimethyl-imidazolium chloride aqueous solution (0.10M)

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References

[1] M. Nagasaka *et al.*, *J. Electrosc. Relat. Phenom.* **200** (2015) 293.

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