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Analysis of Cu K-edge XANES spectra in COMMD6 and COMMD7 with Multiple scattering theory

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Introduction

COMMD6 and COMMD7 are useful proteins that are studied recently for an effect of tumor suppression and they are members of COMMD family. COMMD6 and COMMD7 are composed of 85 and 200 amino acid residues, respectively. Both of them bind Cu ion. Cu ions are supposed to reside in the space between amino acid residues in COMMD family. They are believed to be important for the Cu metabolism. In order to specify the amino acid residues which surround the Cu ion, the multiple scattering analysis of Cu K-edge XAFS spectra is carried out.

Theory

All of XANES spectra are calculated with multiple scattering theory. [1]

Eq. 1 gives the X-ray absorption cross section at site *A*.

$$\sigma = -\frac{8}{3}\mathrm{Im}\left[\sum_{m_c,L,L'} i^{l-l'}\exp\{i(\delta_l^A+\delta_{l'}^A)\}\rho_c(l)\rho_c(l')G(L_c10|L)G(L_c10|L')(t^{-1})_{LL'}^{AA}[(1-X)^{-1}]_{LL'}^{AA}\right] \quad (1)$$

$$X_{LL'}^{\alpha\beta} = t_l^{\alpha}G_{LL'}(\mathbf{R_a}-\mathbf{R_b})(1-\delta_{\alpha\beta})$$

$(1\text{-}X)^{-1}$ accounts for the infinite-time multiple scattering in the model cluster. T-matrix t_l^{α} at site α reflects the electronic state of the X-ray absorbing atom.

Green function GW contains information about the geometrical structure around the X-ray absorbing atom.

Results and discussion

Several structural models for the Cu site in COMMD6 are constructed. Fig. 1 is one of the possible models of COMMD6 (model A), which includes four amino acid residues. The four amino acid residues are arginine, glutamine, leucine and proline, which are chosen by the hydrophobicity-plot of amino acids and the disorder domain projection of COMMD.[2]

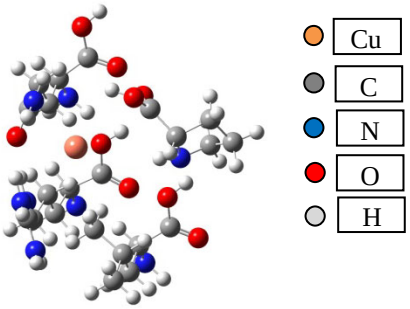

Fig. 1 Calculated model A of COMMD6

Fig. 2 shows the selected results of calculated Cu K-edge XANES spectra for COMMD6 together with the experimental spectrum. The spectrum A corresponds to the above model. The spectrum B is for another model of COMMD which has six amino acid residues at the nearest neighbor of the Cu ion. The first peak (around 8990eV) and the spectral features of between 9000 to 9020eV are strongly influenced by the composition of amino acid residues around Cu ion. The spectrum A shows more resemblance to the experimental spectral features than B around the first peak. Calculations using other possible models are necessary for the determination of the amino acid residues that surround the Cu ion. Extended modeling is under way using the protein structure prediction which can give the information of the stable sites of Cu ion in COMMD. Also EXAFS analysis is now going on, that will give information about the bond length between Cu and neighbor atoms. [3]

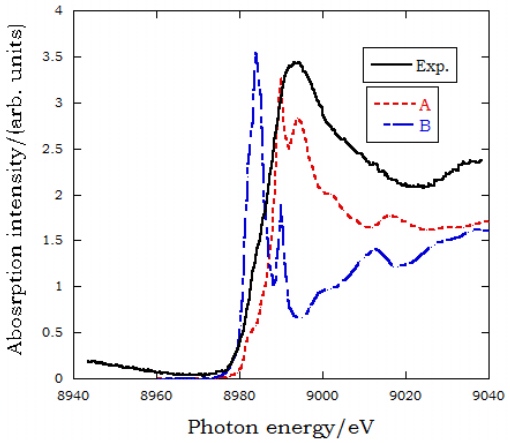

Fig. 2 Cu K-edge XANES spectra of COMMD6

References

[1] T. Fujikawa., J. Phys. Soc. Jpn. **62** (1993) 2155
[2] http://met.bioinfo.pl
[3] H.Taki et al., in this User's report