States and Structures
- Atomic and Molecular Physics -

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Visitors

Prof Kee Hag Lee — Wonkwang University, Korea, 6–12 March, 2002, Korea, 27 September–1 October, 2002
Dr Istvan Cserny — Institute of Nuclear Physics of the Hungarian Academy of Science, Hungary, 25 October, 2002

Scope of Research

The research activities in this laboratory are performed for X-ray structural analyses of biological macromolecules and inorganic materials as follows. The main subjects of the biomacromolecular crystallography are crystallographic studies on the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, and the mechanism of thermostabilization of proteins. In the structural analyses of inorganic materials, the electronic states of atoms and molecules are investigated in detail using conventional X-ray and SR in order to obtain fundamental information on the property and structure of materials. The theoretical analysis of the electronic states and the development of new radiation detectors are also performed.

Research Activities (Year 2002)

Presentations

Structure-based analysis of functional sites of thermostable aspartase, Fujii T, Sakai H, Kawata Y (Tottori), Hata Y, XIX Congress and General Assembly of the Int. Union of Crystallography, 7 - 10 August.

Crystal structures of pokeweed lectins, Hayashida M, Fujii T, Ishiguro M (Kyushu), Hata Y, Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 26 March, Annual Meeting, Prot. Sci. Soc. Jpn., 14 June, Kyushu Symp. on Struct. Funct. Prot. Enzy., 18 July, XIX Congress and General Assembly of the Int. Union of Crystallography, 12 - 15 August, Annual Meeting, Jpn. Biochem. Soc., 16 October, Annual Meeting, Crystallogr. Soc. Jpn., 11 December.

Role of electrostatic interactions in myosin filament formation, Akutagawa T, Hata Y, Ooi T and Katayama E (Tokyo), Annual Meeting, Biophys. Soc. Jpn., 4 November.

X-ray emission spectroscopy around the threshold in 3d and heavy elements, Ito Y, Fukushima S (NIMS), 6th Forum on Superionic Conductor Physics, 15 - 16 May, 19th Int. Conf. on X-ray and Inner-shell Processes, 24 - 28 June, Int. Seminor on Photoionization in Atom, 19 - 20 August, 28th Symposium on Solid State Ionics, 13 - 15 November.

The Mechanism of X-ray emission satellite excited by SR, Vlaicu A. M. (NIMS), Ito Y, Shigeoka N, Oohashi H, Fukushima S (NIMS), Spring Meeting, The Spectro. Soc. Jpn., 16 - 17 May, 19th Int. Conf. on X-ray and Inner-shell Processes, 24 - 28 June, Int. Seminor on Photoionization in Atom, 19 - 20 August. Int. Conf. on the Application and Industry, CAARI 2002, 12 - 16 November.

Grants

Hata Y, Structural investigations of 2-oxo acid:ferredoxin oxidoreductases from archaea, Grant-in-Aid for Scientific Research on Priority Areas (A), 1 April 2001 - 31 March 2003.

Hata Y, X-Ray crystal structure analyses of functional proteins, Grant of Rice Genome Project PR-2202, MAFF, JAPAN, 1 April 2000 - 31 Mach 2003.

Hata Y, Protein-engineering studies on the unique conformations and the expression mechanism of function of pokeweed lectines, Grant-in-Aid for Scientific Research on Priority Areas (C) (2), 1 April 2002 - 31 March 2004.

Hata Y, Structural analyses of gene-products involved in protein structure formation, Protein 3000 Project, 1 April 2002 - 31 March 2007.

Ito Y, For attendance at the international seminar, the Kyoto University Foundation, 2002, Izumi Science and Technology Foundation, 2002.

X-ray crystal structure analysis of pokeweed lectins, PL-D1 and PL-D2

Pokeweed lectin (PL) is a mitogenic lectin, which is specific for N-acetylglucosamine-containing saccharides and exceptionally activates both T and B cells. Five lectins, designated PL-A, PL-B, PL-C, PL-D1, and PL-D2, have been isolated from the roots of pokeweed. Of these lectines, PL-D is the smallest one consisting of two chitin-binding domains, each of which has four S-S bridges and the putative saccharide-binding site. PL-D has two isomers of PL-D1 and PL-D2. PL-D1 comprises 84 amino acid residues and has a molecular mass of 9,317, while PL-D2 has an identical sequence to that of PL-D1 except for the lack of the C-terminal two residues Leu83-Thr84. The crystal structures of PL-D1 and PL-D2 have been solved by the molecular replacement method and refined up to 1.6 Å and 1.5 Å resolutions with the R-factors of 17.5% and 17.6%, respectively. Both PL-Ds have two saccharide-binding sites which are located on one side of the molecule. The relative orientation of the domains is different by 10° in inclination between PL-D1 and PL-D2. The elongated C-terminal two residues in PL-D1 was not observed in the present crystal structure, indicating the flexibility of the region. The C-terminal

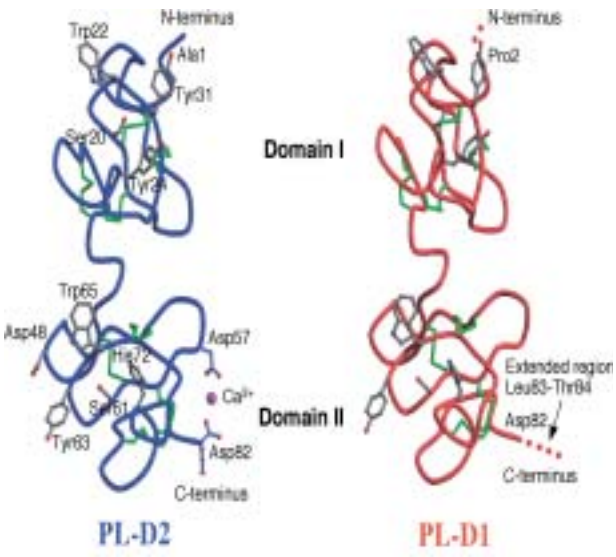

Figure 1. Perspective structures of PL-D1 and PL-D2

α-carboxyl group of PL-D2 binds the Ca^{2+} ion which is coordinated by the β-carboxyl group of Asp57, three water molecules, and the β-carboxyl group of Asp48 from the neighboring molecule in the crystal.

Li K-edge x-ray absorption spectra for lithium compounds

X-ray absorption spectroscopy is expected for a useful method to detect local structure changes and to analyze local quantum structures around Li atoms in various lithium compounds which are studied for developing rechargeable batteries with high capacity.

We have obtained Li K-edge x-ray absorption spectra by electron yield method suitable for the low energy of Li absorption [1]. The results were compared with theoretical spectra and characterized using wave functions which were derived by combination of the molecular orbital and L^2 methods (Fig. 1).

Lithium metal, halides, chalcogenides, oxoacid salts, etc. were studied. Local structure sensitive features and spatial regions of core excitons were revealed. Most of the peaks were assigned to scattering of excited electrons and the characteristic array of the scattering atoms was illustrated for each peak.

1. J. Tsuji et al., *X-ray Spectrometry*, **31**, 319 (2002).

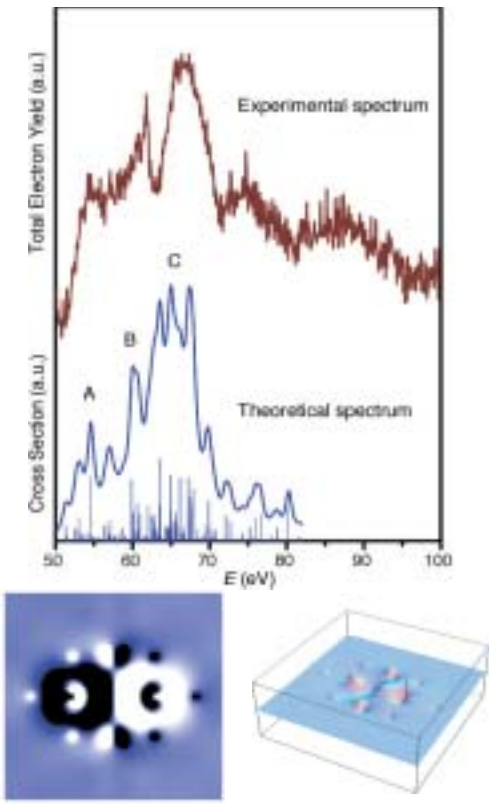

Figure 2. Li K absorption spectra of Li metal and wave functions for the exciton peak of LiF.