Study on the electronic structure of biomaterials using a high efficiency soft x-ray emission spectrometer

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【 Outline of survey 】

Recent progress in crystallization and structural analysis has enabled us to know the three-dimensional structure of main proteins. The origin of biological functionalities is often discussed in terms of these structures. However, it is essential to understand not only the three-dimensional structure but also the electronic structure to elucidate the origin of the biological functionalities. In this study, biological samples like metalloproteins and DNA, are regarded as a material with new functionality, and the origin of the functionality will be clarified by analyzing the electronic structure. Thus the study will contribute to the development in materials science.

We propose soft x-ray emission spectroscopy as a tool to know the electronic structure of biomaterials; it provides information about an element-specific electronic structure; it is applicable to any system, like insulators including biomaterials, regardless of their form such as solution, powder, and so on. On the other hand, there exist technical problems in radiation damage and low signal intensity. New technical development in rapid sample cooling under helium atmosphere, a sample scanning system, etc., will significantly suppress the influence of radiation damage. While development in soft x-ray emission spectrometer, which balances both high detection efficiency and high energy resolution, will allow us to explorer the electronic structure of a reaction center in metalloproteins, where transition metals are included as trace elements.

【 Expected results 】

The knowledge on the electronic structure of metalloproteins and DNA will serve as the physical basis for various applied studies. The electrical property of metalloproteins or DNA can be reflected on the profile around a valence band maximum: a highest occupied molecular orbital (HOMO) state. Moreover, the analysis of a HOMO state serves as an important means that clarifies the details of the chemical reaction. Meanwhile, microscopic information such as charge transfer energy or electron correlation energy, are obtained by using core level spectroscopy.

【 References by the principal researcher 】

Resonant x-ray emission spectroscopy in solids, A.Kotani and S.Shin, Rev. Mod. Phys. **73** (2001) 203-246..

【 Term of project 】 F Y 2004 — 2008

【 Budget allocation 】 73,100,000 yen

【 Homepage address 】 None