

Chem. Commun. **1995**, 655. [2] H. Arzoumanian, L. Maurino, G. Agrifoglio, *J. Mol. Catal. A: Chem.* **1997**, *117*, 471. [3] R.H. Holm, *Coord. Chem. Rev.* **1990**, *100*, 183. [4] J.T. Spence, *Coord. Chem. Rev.* **1983**, *48*, 59.

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Photoinduced conductivity change and structure transformation. Kiyotaka Asakura,^a Takeshi Miyamoto,^a Toshio Naito,^b Yoshinori Kitajima^c ^a*Catalysis Research Center, Hokkaido University, Sapporo, (Japan).* ^b*KEK-IMSS-PF, Tsukuba, (Japan).* ^c*Department of Chemistry, Hokkaido University, Sapporo, (Japan).* E-mail: askr@cat.hokudai.ac.jp

Ag(DM)₂ is a metallic conductor with one-dimensional column. The conductivity and electronic structure are modified by the irradiation of UV Vis light. The electronic conductivity can be controlled from the metallic, semiconductor to insulator region only by the photo-irradiation and thus the Ag(DM)₂ is a promising material for the single material electronic device. We have investigated the origin of the photo-induced conductivity change by Ag K and L_{2,3} edges EXAFS and XANES.

Figure 1 shows the Fourier transforms of Ag K-edge EXAFS. Fig. 1 a shows the pristine Ag(DM)₂. Three peaks appeared corresponding to Ag-N, Ag-(N=), and Ag-(N=C)-N, respectively. Fig. 1 c shows the insulator phase where only one Ag-N distance was found. XRD suggested the amorphous phase was formed. The disorder in the local structure around Ag broke the conduction path to convert the Ag(DM)₂ to insulator. In the other word, the insulator phase was produced by the vitrification of the crystalline structure.

Fig. 1 b shows the semiconductor phase. There are three peaks similar to that in pristine. However, small modifications were found in the first and third peaks. Curve fitting analyses demonstrated that the formation of small number of shorter Ag-N bond. Thus the Ag(DM)₂ molecular structures were collectively modified and small part of the Ag(DM)₂ was involved in the modified structure domains. The boundary between original and modified domains form the conduction barrier for the electron and the semiconductor was formed.

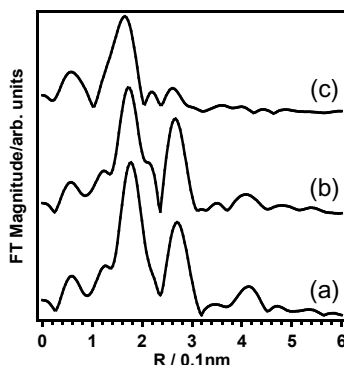


Figure.1 Fourier transforms of (a) pristine conductor, (b) semiconductor and (c) insulator Ag(DM)₂

[1] T. Naito, H. Sugawara, T. Inabe, T. Miyamoto, H. Niimi, K. Asakura, *Molecular Crystals and Liquid Crystals* **2006**, *455*, 311. [2] T. Miyamoto, H. Niimi, W.J. Chun, Y. Kitajima, H. Sugawara, T. Inabe, T. Naito, K. Asakura, *Chem. Lett.* **2007**, *36*, 1008. [3] T. Miyamoto, Y. Kitajima, H. Sugawara, T. Naito, T. Inabe, K. Asakura, *J.Phys.Chem.C* **2009**, *113*, 20476.

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Industrial applications at the national synchrotron light source

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Synchrotron light provides a unique source of non-destructive methods for material characterization. At the National Synchrotron Light Source the industrial program benefits from a large collection of tools to analyze a wide range of materials. Embracing spectroscopic and diffraction methods it is possible to characterize a sample from molecular to atomic levels. Diffraction powder and macromolecular crystallography are typical examples providing useful tools for drug design. X-ray absorption spectroscopy are widely used by our industrial users in their quest to develop better batteries and catalysis studies. Specific examples will be presented and discussed in light of the needs of the industrial researcher.

Keywords: synchrotron, industrial applications, spectroscopy, diffraction

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The particular mechanisms of DNA recognition and dimerization of MITF

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The Microphthalmia-associated Transcription Factor (MITF) is a key regulator of the expression of pigment-cell specific genes in melanocytes, the mature pigment producing cells of the skin and hair follicles. Moreover, in the past few years, MITF became one of the most studied macromolecule in the investigation of the mechanisms leading to melanoma, a particular skin cancer.

MITF is a member of the superfamily of basic Helix-Loop-Helix leucine zipper transcription factors (b-HLH-Zip). Like other b-HLH-Zip factors, MITF can bind a subset of the canonical palindromic E-box sequence (CANNTG) as well as related asymmetric motifs like the M-box (TCATNTG); nevertheless the exact mechanism in which MITF recognizes the correct promoters of target genes is not yet fully elucidated. Within the b-HLH-Zip family, MITF can associate with the Tfe factors, but no heterodimeric complexes containing MITF and the related Myc, MAX or USF-1 have been observed, raising the question how this discrimination is achieved.

We solved three crystal structures: the one of MITF in absence of DNA and two structures of MITF in complex with DNA duplexes encompassing two different target motives (E-box and M-box). In addition, we analyzed interactions between these DNA motives and several MITF mutants with documented phenotypes in mice, using different techniques such as Isothermal Titration Calorimetry, Transactivation assays and EMSA. The comparison of our structural, biophysical and functional data together with available biological data reveals the particular mechanism of DNA recognition by MITF and how MITF discriminates between the E and M boxes. In addition, our data demonstrate an unusual mode of dimerization that might explain how MITF selects its heterodimerization partners.

Keywords: transcription, DNA, interactions.