

BL12B2 NSRRC BM

BL12B2 is one of the two contact beamlines based on the collaborative Memorandum of Understanding between National Synchrotron Radiation Research Center (NSRRC, Taiwan), Japan Synchrotron Radiation Research Institute (JASRI), and RIKEN SPring-8 Center (RSC). The user support and end station maintenance of the beamlines have been provided by NSRRC. BL12B2 has been maintained to serve for material science and protein crystallography users since 2000. The schematic layout of the beamline is presented in Figure 1. The beamline is equipped with collimating mirror (CM), double crystal monochromator (DCM), and focusing mirror (FM). The measured spot size and total flux of the beam is about $250 \mu\text{m}$ square and about 1.5×10^{11} respectively at protein end station at 12 keV. Four end stations, EXAFS, x-ray diffraction, x-ray scattering, and protein crystallography (PX) end stations, are equipped inside the experimental hutch of BL12B2.

The EXAFS experiment is measured using two ion chambers at EXAFS table located at most upper stream of the BL12B2 experiment hutch. The users can carry out experiment by placing their sample in between these two ion chambers. Powder x-ray diffraction is measured using image plate at XRD table located next to the EXAFS table. X-ray scattering experiment can be carried out using six circle diffractometer. The sample environment of these two experiments can be changed from 400 K -20 K using heater and cryostat. High pressure x-ray diffraction can be carried out using CCD camera at protein crystallography table. Protein crystallography (PX) endstation which is equipped with CCD and SPring-8 standard auto sample changer system have been installed since 2009. The user interface software of PX is SPring-8 standard BSS. Remote access capability of this PX system has been tested and operated from 2011.

EXAFS, x-ray diffraction, x-ray scattering end stations are serving for material science users. The experiments are covering wide variety of material science topics, such as environmental science, nano science, geophysical science, etc.

In 2013 BL12B2 users have published nine papers in SCI (Science Citation Index) journals. The material science and protein crystallography users have published three and six papers respectively. Selected results are shown in Fig.2 (material science) and Fig. 3 (protein crystallography). Fig.2 shows

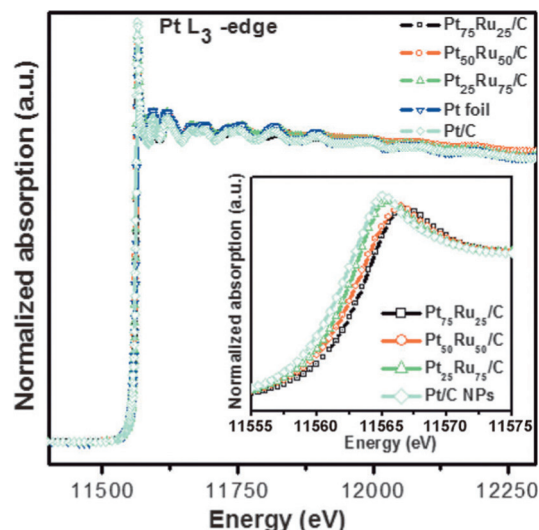


Fig.2 XANES spectra at the Pt L_3 edge for reference Pt foil, Pt/C, and $\text{Pt}_x\text{Ru}_{100-x}/\text{C}$ NPs. The Pt 5d band vacancies for $\text{Pt}_x\text{Ru}_{100-x}/\text{C}$ NPs are lower than the value of the Pt/C NPs. This information suggests that the 5d electron density around the Pt atoms in the $\text{Pt}_x\text{Ru}_{100-x}/\text{C}$ NPs increases owing to partial electron donation from Ru to Pt atoms, owing to hybridization between Ru 4d and Pt 5d states^[1].

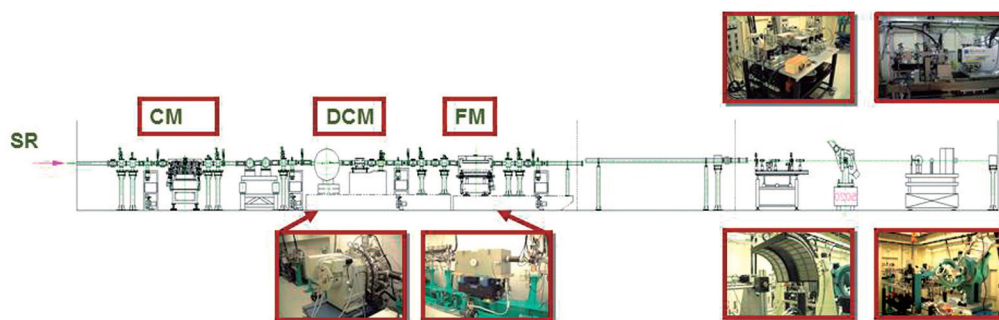


Fig.1 Schematic layout of BL12B2

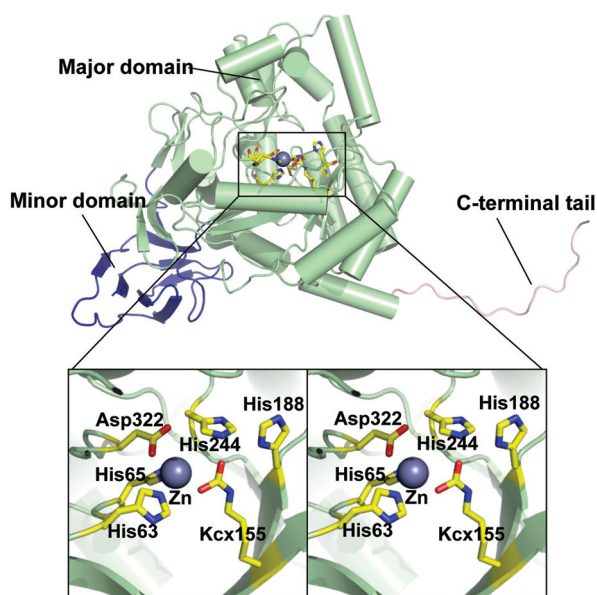


Fig.3 The overall structure of *TnDhp*. The structure comprises three domains: the major domain (green), minor domain (deep blue) and C-terminal domain (pink). The active site is located in the major domain (yellow) (upper panel). The active site with the key residues and zinc atom highlighted in yellow sticks and gray sphere, respectively, is enlarged and shown in a stereo view (bottom panel) [6].

XANES spectra of Pt_xRu_{100-x}/C nanoparticles (NPs) and Pt Foil at the Pt L_3 edge [1]. Fig.3 shows solved crystal structure of *TnDhp* [6].

The beamtime was shared between material science and protein crystallography users with equal amount. The major users of the BL12B2 beamline in 2013 were from Taiwan. There are also international users from Japan and other place of the world. Users support has been provided by three local beamline scientists and one engineer.

Publications

Material Science

- [1] F. Taufany, C.-J. Pan, F.-J. Lai, H.-L. Chou, L. S. Sarma, J. Rick, J.-M. Lin, J.-F. Lee, M.-T. Tang and B.-J. Hwang: "Relating the Composition of Pt_xRu_{100-x}/C Nanoparticles to Their Structural Aspects and Electrocatalytic Activities in the Methanol Oxidation Reaction", *Chem.-Eur. J.* **19** (2013) 905.
- [2] T.-Y. Chen, I.-L. Chen, Y.-T. Liu, T.-L. Lin, P.-W. Yang, C.-Y. Wu, C.-C. Hu, T.-J. M. Luo and C.-H. Lee: "Core-dependent Growth of Platinum Shell Nanocrystals and Their Electrochemical Characteristics for Fuel Cells", *CrystEngComm* **15** (2013) 982.

- [3] A.-J. Chen, I.-J. Hsu, W.-Y. Wu, Y.-T. Su, F.-Y. Tsai and C.-Y. Mou: "A Fluorescent Organic Nanotube Assembled from Novel *p* Phenylene Ethynylene-based Dicationic Amphiphiles", *Langmuir* **29** (2013) 2580.

Protein X-ray Crystallography

- [4] Y.-M. Chang, C. K.-M. Chen, T.-P. Ko, M. W. Chang-Chien and A. H.-J. Wang: "Structural Analysis of the Antibiotic-recognition Mechanism of MarR Proteins", *Acta Crystallogr. D* **69** (2013) 1138.
- [5] Y.-C. Hsieh, T. S. Chia, H.-K. Fun and C.-J. Chen: "Crystal Structure of Dimeric Flavodoxin from *Desulfovibrio Gigas* Suggests a Potential Binding Region for the Electron-transferring Partner", *Int. J. Mol. Sci.* **14** (2013) 1667.
- [6] Y.-C. Hsieh, M.-C. Chen, C.-C. Hsu, S. I. Chan, Y.-S. Yang and C.-J. Chen: "Crystal Structures of Vertebrate Dihydropyrimidinase and Complexes from *Tetraodon Nigroviridis* with Lysine Carbamylation", *J. Biol. Chem.* **288** (2013) 30645.
- [7] Y.-H. Peng, H.-Y. Shiao, C.-H. Tu, P.-M. Liu, J. T.-A. Hsu, P. K. Amancha, J.-S. Wu, M. S. Coumar, C.-H. Chen, S.-Y. Wang, W.-H. Lin, H.-Y. Sun, Y.-S. Chao, P.-C. Lyu, H.-P. Hsieh and S.-Y. Wu: "Protein Kinase Inhibitor Design by Targeting the Asp-Phe-Gly (DFG) Motif: the Role of the DFG Motif in the Design of Epidermal Growth Factor Receptor Inhibitors", *J. Med. Chem.* **56** (2013) 3889.
- [8] M. Maestre-Reyna, W.-J. Wu and A. H.-J. Wang: "Structural Insights into RbmA, a Biofilm Scaffolding Protein of *V. Cholerae*", *PLoS One* **8** (2013) e82458.
- [9] T.-H. Chang, S.-J. Chang, F.-L. Hsieh, T.-P. Ko, C.-T. Lin, M.-R. Ho, I. Wang, S.-T. D. Hsu, R.-T. Guo, W. Chang and A. H. J. Wang: "Crystal Structure of Vaccinia Viral A27 Protein Reveals a Novel Structure Critical for Its Function and Complex Formation with A26 Protein", *PLoS Pathog.* **9** (2013) e1003563.

M. Yoshimura, Y.-F. Liao, T. Tatsumi and H. Ishii
NSRRC, Taiwan