Chemical

Reports on state-of-the-art chemical research conducted at SPring-8 have once again been published in major journals this year, covering research such as the visualization of cathode catalyst layers, single-molecule magnets, the dispersion of single-walled carbon nanotubes using discotic ionic liquid crystals, the application of nuclear resonant vibrational spectroscopy to hydrogenase motion analysis, a pressure-induced structural change of a polymer melt, EXAFS avoiding interference of multielectron excitation effects, and the application of SASE-FEL to study energy transfer in Ar-Ne core-shell clusters.

The X-ray computed laminography-X-ray absorption fine structure (XCL-XAFS) has been developed as a powerful tool to visualize the three-dimensional structural information of catalysts. Prof. M. Tada *et al.* (IMS) revealed, at BL47XU, that the XCL-XAFS technique reveals not only the morphology/structure but also provides three-dimensional structural information on Pt cathode catalyst degradation in a nondestructive manner. Quantum tunneling of the magnetization (QTM) between double-well potentials, which is a prominent property of single-molecule magnets (SMMs), is the basis of high-density storage and quantum computing device concepts. Lanthanoid(III)-phthalocyaninato (Ln(III)-Pc) sandwich complexes behave as SMMs. Prof. M. Yamashita *et al.* (Tohoku Univ.) showed the molecular structure and magnetic relaxation properties of dinuclear Ln(III)-Pc multiple-decker complexes at BL02B1 and BL40XU. A variety of soft electrical conductors have been developed by doping carbon nanotubes (CNTs) into organic and polymeric materials. Liquid crystalline (LC) materials are attracting increasing attention for doping CNTs. Prof. Y. Yamamoto *et al.* (Tsukuba Univ.) found, at BL44B2, that discotic ionic liquid crystals of triphenylene derivatives serve as excellent dispersants for pristine single-walled CNTs.

SCIENCE

The research team of Prof. S. P. Cramer (UC Davis) applied nuclear resonant vibrational spectroscopy to observe Fe-CN and Fe-CO vibrations in the active site of NiFe hydrogenase at BL09XU. Evidence for the liquid-liquid transition in poly(4-methyl-1-pentene) was obtained by high-pressure *in situ* X-ray diffraction measurements at BL10XU. The modest pressures and temperatures at which these phenomena occur are expected to lead to the intriguing possibility of liquid-liquid transitions as industrial processes to control the physical properties of plastics. Ce(IV) is attracting considerable attention in studies of the photocatalytic oxidation of water for producing H_2 and O_2. EXAFS measurements and DFT calculations for identifying the speciation and complex structure of Ce (IV) aquo species in an aqueous acid solution were performed at BL11XU by Dr. Yaita group of JAEA. To avoid problems due to multielectron excitation effects, the XAS spectra were collected at the Ce *K*-edge (40.443 keV). This also enabled EXAFS spectra to be obtained over a wider *k*-range, providing a higher spatial resolution. A research team led by Prof. Ueda (Tohoku Univ.) and Prof. Yao (Kyoto Univ.) found that more than 90% of the energy absorbed by the Ar core was transferred to the Ne shell in the photoionization of Ar-Ne core-shell clusters by SASE-FEL radiation. Preferential energy injection into the Ar core results in ionization dynamics characterized by a charge transfer from the core to shell. This kind of large energy transfer may be useful for reducing the influence of Coulomb explosion of bio-molecules during X-ray diffraction experiments using X-ray lasers.

The continuing improvement in the emittance of the SPring-8 storage ring, the brightness available from improved undulators, and the stability of the high-resolution X-ray monochromators have all contributed to making the above work possible.

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