Chemical


"Hanabishisou"- *California poppy*

Many excellent articles have been published this year by SPring-8 users in this Chemical Science category, covering research areas including FEL applications, atomic and molecular spectroscopy, porous coordination networks, metal-organic complexes, liquid structures, and catalysts. Some representative topics are selected as follows.

In the field of atomic and molecular spectroscopy, the first topic highlighted here is the first observation of free-electron-laser-induced collective spontaneous emission (superfluorescence). The process was observed in He gas using the extreme ultraviolet FEL pulses of the RIKEN SCSS. In the second topic, interatomic electronic decay processes in rare gas dimers NeAr and Ar_2 have been investigated using electron-ion-ion coincidence momentum-imaging techniques at BL27SU by Prof. Ueda *et al*. (Tohoku Univ.). Three-electron interatomic Coulombic decay (ICD) and electron-transfer mediated decay (ETMD) phenomena were observed for the first time.

In the field of large scale molecular networks, Prof. S. Kitagawa *et al*. (Kyoto Univ.) used a four-circle diffractometer at BL13XU to demonstrate a crystal extractor based on porous coordination polymers with core-shell heterostructures. In this system the storage container is the core crystal, and the size separation filter is the shell crystal. In addition, it was demonstrated at BL02B2 and BL19B2 that "instant synthesis" can form kinetic microcrystalline porous coordination networks suitable for *ab initio* XRPD structure determination, and also how new porous structures could be obtained by the annealing of kinetic products. Synthetic methods for multi component metal-organic complexes (molecular spheres) using self-assembly of transition metal ions and bidentate ligands were developed, and synchrotron X-ray diffraction studies were applied to determine their single crystal structures at BL38B1.

SCIENCE

Interesting new information on liquid structures has been obtained at BL04B2 and BL08W. A better understanding of the origin and the extension of nanoheterogeneities in ionic liquids is a crucial step towards a better comprehension of their unusual properties. Studies combining high-energy synchrotron X-ray diffraction (BL04B2) with atomistic molecular dynamics simulations were carried out to explore the atomic structure of imidazolium-based ionic liquids with three different alkyl chain lengths. The possibility of designing a liquid adapted to a particular application by combining appropriate cations and anions was revealed. In related work, in order to characterize hydrogen bond and solvation structures in ethanol-water mixtures at various alcohol concentrations, X-ray Compton scattering experiments were carried out at BL08W, and inhomogeneities in alcohol-water systems were found. This study demonstrated the power of X-ray Compton scattering for studying the detailed geometrical properties of liquids.

In the catalysis field, a joint group from Kyushu University and Hokkaido University used CuPd bimetallic alloy nanoparticles to perform reduction of NO_3^- into NH_3 with photocatalytically-generated hydrogen, an environmentally-benign process that could produce NH_3 without releasing CO_2 and consuming excess energy. In this study, it was found that photocatalytically-generated hydrogen exhibits high selectivity for conversion of NO_3^- to NH_3. The CuPd alloy structure was analyzed using XRD techniques at BL44B2. A research team from the Institute for Molecular Science has succeeded in scanning μ-XRF and μ-XAFS measurements of a single catalyst particle of $NiO_x/Ce_2Zr_2O_y$ ($0 \leq x \leq 1$, $7 \leq y \leq 8$), which is known to exhibit high oxygen storage/release properties and is thus expected to become a highly important automobile exhaust catalyst. The experiments used an X-ray μ-beam (1000 nm (h) × 800 nm (v)) at BL37XU. Use of the μ-XAFS technique will provide structural information of each catalyst particles with different catalytic behaviors, and contribute to the development of more precise catalyst design for chemical reactors.

Yuden Teraoka