Chemical Science

Chemical Science involves various studies including soft matter for devices, nanoparticles, reaction mechanisms, and properties of atoms, molecules and clusters. Soft matter is often composed of organic molecules with a large molecular weight which are bound together through van der Waals interaction. It can be characterized by flexibility, lightness and diversity. Poly[(R)-3-hydroxybutyrate] fibers are bio-based and biodegradable structure plastics. Micro-beam X-ray diffraction at BL47XU revealed that these fibers have a core-sheath structure. The application of soft matter to electronic and magnetic devices draws much attention because it can replace heavy and rigid inorganic semiconductors. The structure of the single component molecular metal, [Au(tmdt)$_2$], which has unique electronic and magnetic properties, has been determined by a powder X-ray diffraction method at BL02B2. The color of the dye in crystal and aggregate is not determined only by molecular structure but by intermolecular interaction. The structure of J-aggregates at the air/water interface has been determined by grazing incidence X-ray diffraction at BL46XU. The origin of the change in the color of J-aggregates comes from the interaction of both TDS (transition dipole moment) and EDM (electric dipole moment). Metal-organic hybrid compounds are another interesting material. They often form a pore structure. Cu(II) *trans*-1,4-cyclohexanedicarboxylate (Cuchd) was studied using powder X-ray diffraction method at BL02B2, and showed that anomalous structural phase transition and toluene adsorption suppress phase transition. [$Cu_2(pzdc)_2(pyz)$] can adsorb C_2H_2 selectively and can separate it from coexisting CO_2. The powder diffraction revealed that the hydrogen bonding of C_2H_2 with free oxygen atoms fixed C_2H_2 molecules in the pore in 1D channels. Fundamental studies of atoms, molecules and clusters are important in nanoscience. Symmetry resolved high-resolution photoelectron spectra of CO and N_2 were measured at BL27SU and the fine structures in the satellite were found to arise from vibrational modes in excited molecules. Another interesting paper from BL27SU is that on the electronic structure of hydrogen-bonding clusters which must be the base for understanding of solvation and protonation in liquid chemistry. Bimetallic nanoparticles are important in catalysts and optical materials. A new means of classifying the inner structure of bimetallic nanoparticles by EXAFS at BL12B2 has been proposed and the structure of PtRu has been determined. Last but not least, important progress has been made from IR beamline BL43IR, which showed pseudo gap formation in CdSb under multiple extreme conditions (i.e., high temperature, high pressure and high magnetic field).

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