Chemical

Target materials of *Chemical Science* widely spread from simple molecules to complex biosystems across different length scales. Synchrotron X-ray diffraction analysis combined with complementary spectroscopic techniques such as XAFS and NRVS (nuclear resonance vibrational spectroscopy) provide the fundamental structure of simple molecular solids/liquids and a full three-dimensional picture of the hierarchical structure of complex materials. Precise and accurate structural study is essential for understanding the functional properties and mechanisms of these materials in combination with the electronic states studied by PES and XES with a synchrotron light source as well. The trend in Chemical Science studies is going toward dynamics study as demonstrated by the topics collected in *Research Frontiers 2008*. Their outlines are summarized below.

The structure of liquid water has been the issue in materials sciences during the past century. X-ray emission study on the liquid structure provided definite evidence of the coexistence of two species, fourfold and less than fourfold hydrogen-bonded structures, which supports a two-component model. Molecules exhibit a peculiar configuration in the liquid phase even for simple diatomic molecules such as N_2 and O_2. X-ray diffraction measurement at high pressures revealed that diatomic linear molecules tend to take mutually parallel and X-shaped configurations in dense-liquid states as a result of the strengthening of intermolecular interactions. Precise structural study is essential for understanding the distinct behavior of mixed-valence one-dimensional metal chains. Single-crystal X-ray diffraction measurement determine the Pt-Pt distances accurately and allow the average oxidation number of Pt atoms in Pt-Pt chain compounds. The structural study of ionic liquids is a hot topic in chemistry and chemical engineering. A detailed analysis of high energy X-ray and neutron diffraction data reveals that the dominant chain structures consisting of several atoms joined by hydrogen bonding in the liquid state of $Cs(FH)_{2.3}F$, which are not observed in the solid state. The biological nitrogen fixation in microorganisms is investigated by EXAF and NRV. A Fe_6S_9 cage with an interstitial atom is shown to play a key role in the fixation. Selective chemical bond breaking or control of chemical reaction is attempted by ionizing of a target core using well-tuned soft X-rays. *Ab initio* structural determination from powder diffraction data is expanded to medium-size pharmaceuticals.

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SCIENCE