Visiting Professors

Visiting Professor
ABE, Manabu *(from Hiroshima University)*

Stretch Effects Induced Molecular Strain in Generating Long-Lived Biradicals

Stretch effects induced by two types of molecular strain were examined by quantum chemical calculations, to design persistent multi-radicals such as localized diradicals and oxyallyls. The cooperative molecular strain (Type-1) induced by the spiro[5.5]undecane and bicyclo[2.1.0]cyclopentane structures was found to significantly destabilize in energy the ring-closed compounds of the diradicals, leading to small energy differences between the diradicals and the σ-bonded compounds. Another stretch effect (Type-2) induced by macrocyclic systems was also found to energetically destabilize the corresponding ring-closed structures of the 1,3-diradicals. The computational studies predict that the two types of stretch effects are quite effective in lowering the energy barriers of the bond-breaking reaction of the ring-closed compounds and in generating long-lived localized diradicals and oxyallyl derivatives.

Visiting Professor
KATO, Tatsuhisa *(from Kyoto University)*

Studies of Molecular Magnetization of Super-Molecules

The encapsulation of C_{60} with γ-cyclodextrin (γ-CD) has been attained by a mechanochemical high-speed vibration (HSV) technique. N@C_{60}, which can be a good magnetic probe giving the information of position as well as of chemical environment, should be soluble in water for the purpose of biological application. Then the HSV technique was applied to the powder of γ-CD and C_{60} containing N@C_{60} at 5%. The obtained molecular complex exhibited the peculiar electron spin resonance (ESR) spectrum of N@C_{60} in water.

We designed the flexible intermolecular communications in a simple molecular architecture by using mechanically interlocked supramolecular motives such as catenanes and rotaxanes, in which two or more molecular components are inseparable but their interactions are flexibly convertible. In a dinuclear Cu^{2+} complex of the four-fold rotaxane, the Cu^{2+}-porphyrin and the Cu^{2+}-phthalocyanine were stacked efficiently on one another to afford spin–spin communication. Spin states of the dinuclear complex were switchable between its protonated form (doublet) and deprotonated form (singlet) reversibly.

Visiting Professor
ASAKURA, Tetsuo *(from Tokyo University of Agriculture and Technology)*

Determination of Molecular Structure with Ultra Fast MAS under High-Field NMR

In single crystal X-ray diffraction analyses of peptides and proteins, it is well-known that the co-ordinates of carbon, nitrogen and oxygen atoms can be obtained in high accuracy, but enough accuracy cannot be obtained for those of hydrogen. Therefore we are trying to determine the accurate ^{1}H positions by the combination of NMR observation by ultra fast magic angle spinning under high field magnetic field and accurate ^{1}H NMR chemical shift calculation. We are applying this novel analytical technique to determine the structures of silk fibroins before and after spinning together with their model peptides. Since such a ^{1}H information is sensitive to both the intra- and inter -molecular structures, it is especially useful in molecular design of biomaterials with silks.