

Newly Designed Website for SPring-8 Users

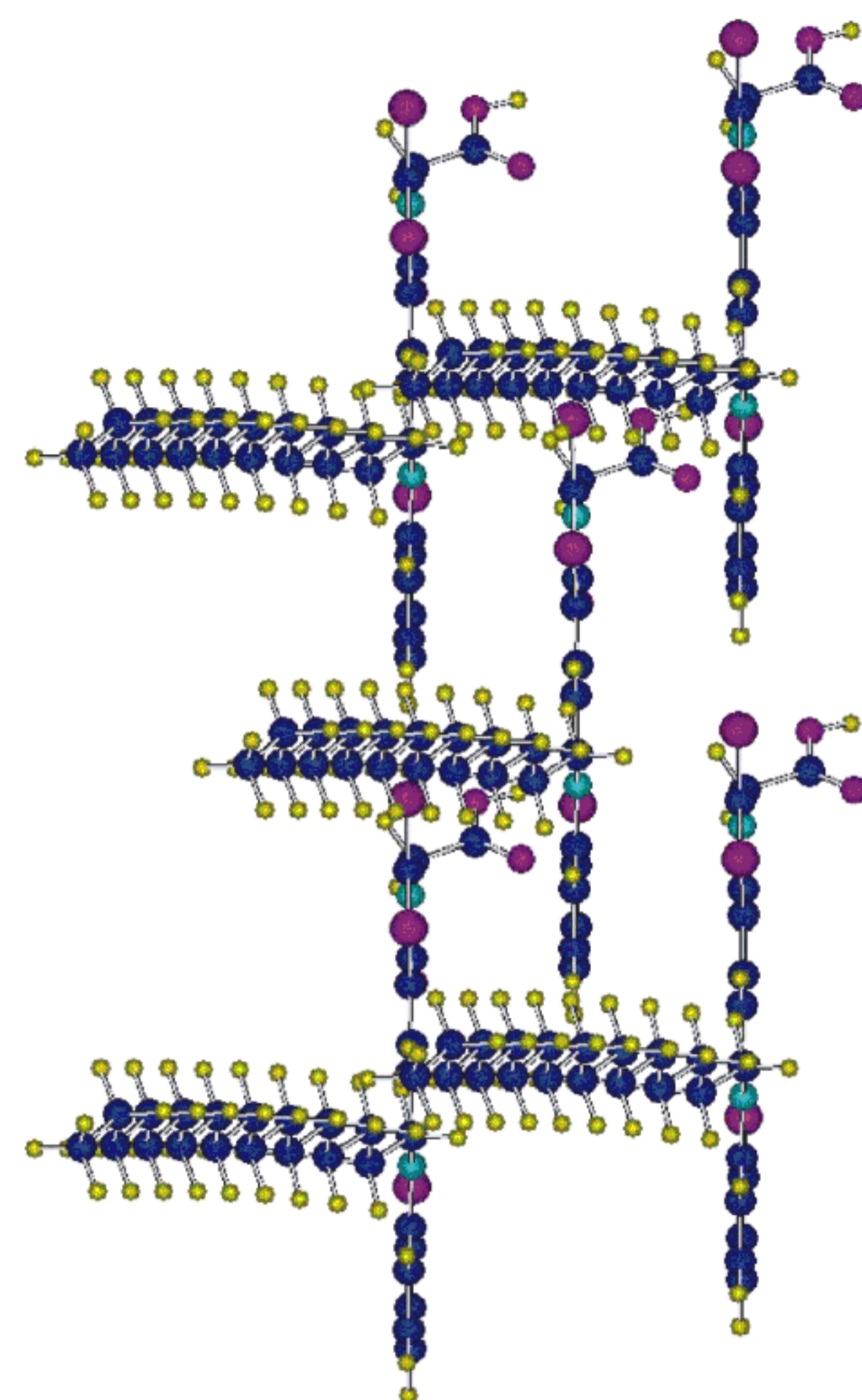
The SPring-8 User Information Website:  
<http://user.spring8.or.jp/en/>

## Relation between the crystal structure and the crystal color of organic dye molecules

Drs. N. Kato, K. Yuasa (Waseda Univ.), Mr. T. Araki (Waseda Univ.), Prof. Y. Uesu (Waseda Univ.), Drs. I. Hirosawa, M. Sato, N. Ikeda (JASRI/SPring-8), and Dr. K. Iimura (Utsunomiya Univ.) succeeded in determining the structure of the two-dimensional crystal of the organic dye molecules and quantitatively clarified the relation between the crystal structure and the crystal color, using a grazing incidence X-ray diffraction method at the R&D Beamline, BL46XU [Phys. Rev. Lett. 94, 136404 (2005)].

In general, the color of organic dye molecules changes upon crystallization. When the visible absorption peak shifts to longer wavelength upon crystallization, such crystals are called J-aggregates. Amphiphilic merocyanine (MC) dye molecules form a monolayer consisting of J-aggregates (two-dimensional crystals) at the air-water interface, and turn the color from red to blue upon crystallization. And in order to provide quantitative explanations for the peak shift (color change), the complete crystal structure had to be clarified.

The calculation based on the determined structure revealed that the electric dipole interaction, which had not been taken into account so far, made a significant contribution to the exciton band wavelength. In the calculation, they derived and used simple formulas for the electric dipole interaction energy and the transition dipole moment interaction energy. The formulas, utilized to estimate the structure or the color of the molecular crystals and aggregates, will be useful for developing and designing the optical devices based on the organic dye molecules.



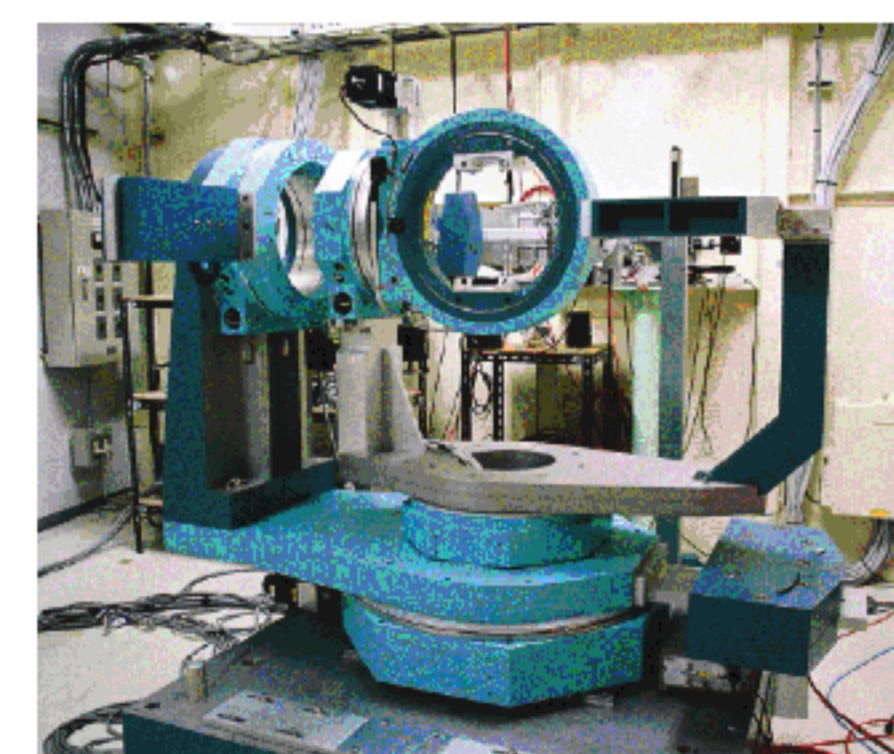
Molecular arrangement on the 2D base-centered unit cell of the merocyanine J-aggregate

## R&D Beamline, BL46XU

This X-ray undulator beamline has been dedicated to R&D activities for the SPring-8 staff, including insertion device R&D. At the beamline, the hybrid undulator consisting of 186 magnets with the short undulator period of 24 mm is installed at present. The photon energy from 12 to 25 keV can be obtained with a combination of the fundamental undulator peak and the Si 111 reflection. In the experimental hutch, the multi-purpose diffractometer with standard four circle axes ( $\chi$ ,  $\phi$ ,  $\omega$  and  $2\theta$ ) and four additional axes is installed, and is controlled using the SPEC program.



Drs. M. Mizumaki (left) and S. Kimura (right)  
[Beamline Scientists]



Multi-purpose diffractometer

### XRM 2005

The 8th International Conference on X-ray Microscopy, XRM2005, will be held at the Egret Himeji, Hyogo, Japan, from July 26 to 30, 2005.

<http://xrm2005.spring8.or.jp/>

### SRI 2006

The 9th International Conference on Synchrotron Radiation Instrumentation, SRI 2006, will be held at the EXCO Center, Daegu, Korea, from May 28 to June 3, 2006.

<http://sri2006.postech.ac.kr/>