Femtosecond structure determination of molecules in an alignment laser by photoelectron diffraction with a XFEL

S. Minemoto[1], T. Teramoto[2], H. Akagi[3], T. Fujikawa[4], T. Majima[5], K. Nakajima[6], K. Ogawa[7], H. Sakai[1], T. Togashi[6], K. Tono[6], S. Tsuru[4], S. Yoshida[5], K. Wada[8], M. Yabashi[7], and A. Yagishita[8]

[1] *Graduate School of Science, The University of Tokyo, Bunkyo-ku, Tokyo, Japan*
[2] *College of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga, Japan*
[3] *Quantum Beam Science Center, Japan Atomic Energy Agency, Kizugawa, Kyoto, Japan*
[4] *Graduae School of Science, Chiba University, Chiba, Japan*
[5] *Graduate School of Engineering, Kyoto University, Katsura, Kyoto, Japan*
[6] *Japan Synchrotron Radiation Research Institute, Sayo, Hyogo, Japan*
[7] *RIKEN SPring-8 Center, Sayo, Hyogo, Japan*
[8] *Institute of Materials Structure Science, KEK, Tsukuba, Ibaragi, Japan*
E-mail: minemoto@phys.s.u-tokyo.ac.jp

Abstracts: *We have successfully measured the X-ray photoelectron diffraction (XPD) of laser-aligned iodine molecules by using X-ray free electron laser pulses. Thanks to a higher degree of alignment of sample molecules, we have obtained the XPD image having structural information. The experimental XPD image is analyzed with the help of the XPD theory to obtain the structure of molecules in an intense laser field.*

In the last two decades, laser-induced alignment and orientation techniques of molecules are well developed and successfully applied to high-order harmonic spectroscopy [1], photochemical reaction controls [2], and so on. However, a fundamental aspect of the technique was not scrutinized so far; the intense field of the alignment pulse may modify the ground-state structure of the molecules, especially in the case of the adiabatic alignment technique. Here we report our recent results on the structure determination of iodine molecules, I_2, in an intense laser field by the X-ray photoelectron diffraction (XPD) using ultrafast X-ray Free Electron Laser (XFEL) pulses [3,4].

The experiment was performed at BL3 of the SACLA facility with the photon energy of 4.7 keV. The momentum images of both electrons and ions produced by the XFEL pulses have been measured simultaneously with double velocity-map imaging spectrometers [3]. The sample I_2 molecules are aligned parallel to the polarization direction of XFEL by the Nd:YAG laser pulses. The degree of alignment was estimated to be ~0.73 from the obtained fragment-ion images.

The measured electron image consists of the central part for low-energy electrons due to Auger cascades and the outer ring of I 2*p* photoelectrons with kinetic energy of 140eV, i.e., the XPD image. Thanks to the higher degree of alignment compared to that in [3], we have observed intensity minima in the XPD as shown in Fig. 1, though interference structures could not be resolved. To determine the molecular structure, i.e., the bond length of the I_2 molecules in the Nd:YAG laser field of ~1x10^{12}W/cm^2, we have applied our molecular-structure-determination methodology [4] to the measured XPD data. Thus, we have found that the bond length in the laser is longer by 0.5Å than the equilibrium nuclear distance. The details of the present work will be discussed in the presentation.

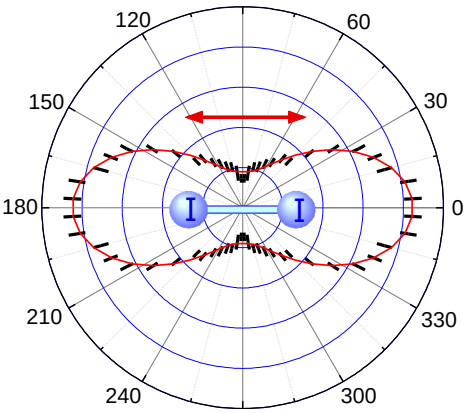

Fig. 1: Angular distributions of I 2*p* photoelectrons. The arrow shows the polarization direction of XFEL pulses.

[1] T. Kanai, S. Minemoto, and H. Sakai, Nature (London) **435**, 470 (2005).
[2] M. D. Poulsen *et al*., J. Chem. Phys. **117**, 2097 (2002).
[3] K. Nakajima *et al*., Sci. Rep. **5**, 14065 (2015).
[4] M. Kazama *et al*. Phys. Rev. A **87**, 063417 (2013).