Application of photoelectron diffraction theory to ultrafast molecular dynamics

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X-ray free electron laser (XFEL) offers the possibility of diffractive imaging of small objects within a few femtoseconds. Irrespective of whether the diffraction is due to the detection of photons or photoelectrons, it is required that the measurement is done in the reference frame of the molecule. Here we propose a new scheme of ultrafast photoelectron diffraction (UPD), which is based on (1) upcoming XFEL, (2) molecular frame inner-shell photoelectron diffraction images, and (3) reconstructions of them by multiple-scattering theory [1]. Ultrafast molecular dynamics induced by a pump pulse will be obtained as the photoelectron diffraction images, which encode the molecular structure at the instant of XFEL photoionization. To examine the validity of the scheme, we have performed multiple scattering calculations for oriented H_2O molecules and oriented NO_2 molecules. The molecular geometries are taken as parameters in the calculations. The results have been compared with experimental data, which had been measured using coincidence technique [2], and the residual error (R) has been evaluated.

For O 1s 90 eV photoelectron from H_2O molecule, the minimum R was obtained when the bond angle is 114° and the bond length is 1.00 Å. Figure 1 shows the experimental and calculated angular distributions for H_2O, O 1s 90 eV photoelectron. The solid line shows the calculated result for the minimum R.

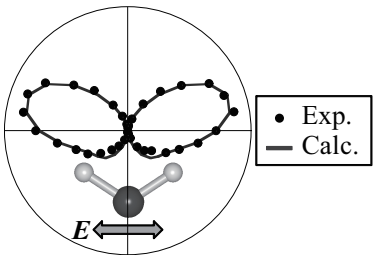

Figure 1: Experimental result and calculated result when R takes the minimum for O 1s photoelectron from H_2O molecule. The kinetic energy of photoelectron is 90 eV. X-ray polarization vector $\boldsymbol{E}$ and molecular orientation are shown.

The results for NO_2 will be also reported. These results demonstrate the promising outcome of UPD: The molecular structural parameters can be determined by estimating R factor.

Reference

[1] M. Kazama, *et al.*, Chem. Phys. 373 (2010) 261.

[2] A. Yagishita, K. Hosaka, J. Adachi, J. Elect. Spect. Relat. Phenom. 142 (2005) 295.