Probing Electron Momentum Densities of Molecular Orbitals Using New Multichannel (e,2e) Spectrometers

Masahiko Takahashi

Institute of Multidisciplinary Research for Advanced Materials,
Tohoku University, Sendai 980-8577, Japan
(masahiko@tagen.tohoku.ac.jp)

Electron momentum spectroscopy (EMS), based on the binary (e,2e) reaction under the high-energy Bethe ridge conditions, has been developed as a powerful means for investigating the electronic structures of atoms and molecules [1]. In particular, its unique ability to look at individual electronic orbitals in momentum space has been widely exploited in the last three decades with the aid of the plane-wave impulse approximation. Nevertheless, the potential of EMS has not been fully achieved for molecules as yet due mainly to the small cross sections involved and the fact that the experiments measure averages over all orientations of gaseous targets. Spherical averaging results in enormous loss of versatile information on collision dynamics and electronic structure; three-dimensional character of the (e,2e) scattering by molecules deteriorates into the one-dimensional momentum distribution or momentum profile.

Very recently, we have developed two types of multichannel (e,2e) spectrometers [2,3]. The first spectrometer [2] measures conventional (e,2e) cross sections, but it features remarkably high sensitivity by simultaneous detection in energy and momentum. The second spectrometer [3] has been developed for examining (e,2e) reactions in the molecular frame. In the axial-recoil limit of fragmentation of the residual molecular ion, measurements of vector correlations between the two outgoing electrons and the fragment ion are equivalent to (e,2e) experiments with fixed-in-space molecules.

In this contribution we report details and performances of the newly developed spectrometers. Our recent studies on several targets will also be presented. Applications to be discussed will involve the first observation of anisotropy of molecular frame (e,2e) cross section [3-5]. We will demonstrate a geometry effect of molecular orientation on the (e,2e) amplitude and how it depends on the nature of the final ion state.

References

[1] E. Weigold and I.E. McCarthy, *Electron Momentum Spectroscopy* (Plenum, New York, 1999).
[2] M. Takahashi, T. Saito, M. Matsuo, and Y. Udagawa, *Rev. Sci. Instrum.* **73**, 2242 (2002).
[3] M. Takahashi, N. Watanabe, Y. Khajuria, K. Nakayama, Y. Udagawa, and J.H.D. Eland, *J. Electron Spectrosc.* **141**, 83 (2004).
[4] M. Takahashi and Y. Udagawa, *J. Phys. Chem. Solids.* **65**, 2055 (2004)
[5] M. Takahashi, N. Watanabe, Y. Khajuria, Y. Udagawa, and J.H.D. Eland, *Phys. Rev. Lett.*, in press.