Giant resonance in 4d photoionization of Xe-like isoelectron sequence

M. Sato[1)], X. M. Tong[2)], T. Watanabe[1,2)]

[1)] *Physics Department, International Christian University, Mitaka, Tokyo 181-8585, Japan*
[2)] *Cold Trapped Ions Project, ICORP, JST, Axis 3F, 1-40-2 Fuda Chofu Tokyo 182-0024, Japan*
Tel: +81-0424-83-1094, Fax: +81-0424-83-1409

Giant resonance in rare-gas photoionization process has been a subject of interest for a long time [1, 2]. The broad resonance of 4d electron photoionization cross section for rare gas atoms can be explained as being due to the electron-electron dynamic correlation and the double-well potential for the final f partial wave [2]. Although the giant resonance in the rare-gas atom has been extensively studied, the behavior of the photoionization of rare-gas-like atomic ion is not so well studied. Based on linear density response theory with an optimized effective potential method and a self-interaction correction [3, 4], we have studied the giant resonance of 4d photoionization in Xe, Cs^+ and Ba^{2+} atomic ions. Generally speaking, the shape of the photoionization (or photo-excitation) cross section is related to two interactions. One is electron-electron interaction which may result a giant resonance. Another is electron nucleus interaction which results a monotonic decrease behavior. In the experiments, a broad 4d giant resonance far above the ionization threshold for Xe atoms is observed. The 4d giant resonance moves close to the ionization threshold for Cs^+ and then moves below the ionization threshold for Ba^{2+}. The photoionization (photoexcitation) cross section of higher charged ions decreases monotonically as the photon energy increases due to electron-nucleus interaction becomes dominant. Based on our calculated results, we can illustrate the evolution of the 4d giant resonance of Xe-like iso-electron sequence as: (1) the width of the giant resonance is narrower for higher ionization degree atoms; (2) the resonance peak is moving to the leading state of the final channel; (3) the resonance peak is merged with the leading state of the final channel when the electron-nucleus interaction is dominant (H-like photoionization behavior). [Note that the electron configuration will changes for higher ionization degree, which does not happen for Ba^{2+} yet.] If the giant resonance moves below the ionization threshold, the photo-excitation cross section will be enhanced dramatically. In the experimental observations, we found that the photo-excitation cross sections are very small in Xe case and the photo-excitation cross sections [4] are almost in the same magnitude as the above threshold resonance for Cs^+ atoms [5]. The photo-excitation cross sections are much larger than that of the photoionization process in Ba^{2+} case [6]. All such experimental observations are well reproduced in our calculations. Furthermore, we can decompose different final partial wave contributions in photoionization (or photo-excitation) process by selecting a special final channel partial waves. By decomposing different partial waves contribution, we can sign the photo-excitation peaks observed in the experiment.

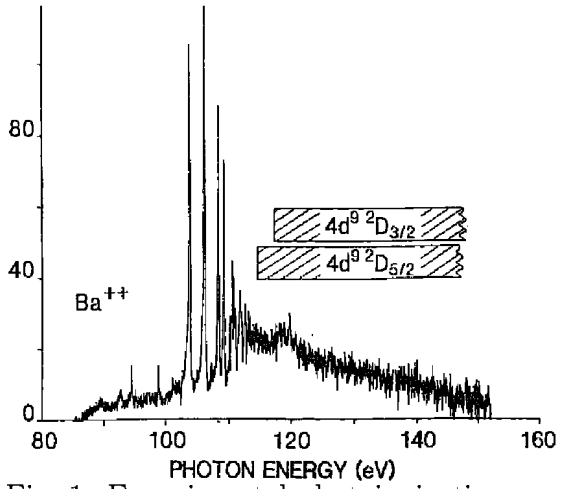

Fig. 1. Experimantal photoionization cross sections of 4d electrons from Ba^{2+}.

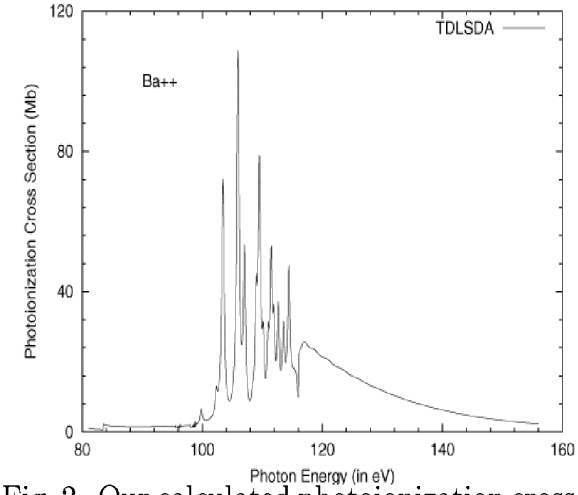

Fig. 2. Our calculated photoionization cross sections of 4d electrons from Ba^{2+}.

As an example, we show the experimental spectra [6] in Fig. 1 and our calculations in Fig. 2 for Ba^{2+}. To compare with the experiment, the experimental width (or energy resolution) is used in the linear density response calculation. Since our calculation is based on the non-relativistic density functional theory, the fine structure split of 4d orbital is not taken into account in the calculation. To compare with the experiment, we shift the calculated spectra by 2.5 eV (fine structure splitting of the 4d orbits) and sum them up with a statistical weight. The final spectra totally shifts 4 eV due to the energy difference of our calculated 4d orbital energy with the experimental one. Our final folding spectra is in reasonable agreement with the absolute experiment results both in the general shape and the detail auto-resonance peaks as shown in Fig 1 and Fig. 2. The detail discussion will be appeared elsewhere [7].

To summary, we have studied the 4d photoionization and photo-excitation process in the Xe-like iso-electron sequence by the linear density response method. The calculated results are in reasonable agreement with the experiments. By decomposing the contribution of the final partial waves, we can assign the auto-resonance peaks observed in the experiments.

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