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钠原子激发态 2p 内壳层光电离过程的伴线结构

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摘要: 基于多组态 Dirac-Fock 方法, 理论研究了钠原子 2p 光电离过程高分辨率的光电子谱及振激跃迁过程的相应伴线谱。展示并解释了正常光电离和强振激跃迁过程相应光电子谱的主要特征; 结果表明光电离后 2p 空穴的电子关联在一定程度上改变了相应谱线的能量位置, 对出射光电子谱的结构有很大影响。实验测量与理论模拟谱之间的一致性说明了该理论方法的可靠性, 从而能够正确辨认相应的实验观测谱线。

关键词: 光电子谱; 振激; 多组态 Dirac-Fock 方法; 电子关联; 弛豫

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Photoelectron Satellite Structure from the 2p Inner-shell Photoionization of Excited Sodium Atoms

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Abstract: Based on multiconfiguration Dirac-Fock method, the high-resolution 2p photoelectron spectra and satellites originating from the corresponding shakeup transitions during the photoionization of neutral sodium atoms are theoretically studied. The main features of photoelectron spectra from the normal photoionization and strong shake-up transitions are presented and interpreted. It is shown that the electron correlations of the 2p hole affect the energy positions of photolines and give rise to considerable structures in the photoelectron spectra. The reasonable agreement between the measured results and simulated spectra confirms the reliability of the theoretical approaches and enables us to assign the observed photolines.

Key words: Photoelectron spectra; Shake-up; Multiconfiguration Dirac-Fock; Electron correlation; Relaxation

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0 Introduction

Photoionization, i. e., the emission of an electron after the absorption of a photon, is one of the most

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fundamental atomic processes in light-matter interactions, which has been studied for many years^[1-2]. Thus, the photoelectron spectrum is a well-established method for studies of atomic structures in various forms of matter and is a powerful tool for estimating element abundances^[3-4]. Moreover, rapid developments in the technology of modern light sources and the emergence of high-precision detectors have enabled experimentalists to obtain very accurate data on photoionization processes, and experiments on atomic photoionization have become possible by utilizing the high photon flux of third-generation synchrotron radiation sources, the photon-ion merged-beams technique^[5] and free electron lasers^[6], thereby facilitating measurements with unprecedented sensitivity and resolution.

In most cases of inner-shell photoionization, the photoion will be left in a final hole state, where only one of the electrons is removed from the initial configuration. Much less likely, however, it is the formation of a final state of the photoionization system, which is associated with an excitation of one additional electron. Such photoionization with excitation requires a correlated motion of the electrons, and the corresponding transition matrix element will be nonzero only if the electron-electron interaction is taken into account^[7-8]. From the shake theory^[9], shake-up satellites arise in the sudden approximation, where the photoionization causes a sudden change in the Coulomb attraction, i. e., in addition to the photoemission of an inner-shell electron, a rearrangement of the residual electron density is likely to occur and leads to a satellite structure to the main photoelectron peaks. The 2p photoionization of excited and ground states of sodium atoms has been experimentally investigated using synchrotron radiation, and the corresponding analyses were performed with different approximations, such as many-body perturbation and multiconfiguration Hartree-Fock methods, and the results revealed the strong influence of electron correlation^[1,8,10]. It was observed that the shake-up process becomes more probable than the single photoionization as the principal quantum number of valence electrons increases^[11]. The different spectrum structure arising from single photoionization and photoionization accompanied by excitation, i. e., satellite photoelectron structure originating from the corresponding shake-up transitions during the 2p photoionization, were observed^[12]. Motivated by the experimental photoelectron spectra, we performed a detailed Multiconfiguration Dirac-Fock (MCDF) calculation to understand the spectrum structure from the shake-up transitions during the 2p photoionization from excited states of sodium atoms. In this paper, the focus is on how shake-up satellites appear in the photoionization process by explicitly treating the electron correlation between photoelectrons and photoions. Atomic units are used throughout the paper unless otherwise specified.

1 Theory

For open-shell atomic structures, the MCDF method has been found to be a very versatile tool for calculating photoionization cross sections and binding energies^[13-14]. In this method, the Atomic State Functions (ASFs) of interest are generated as linear combinations from the relativistic jj coupled Configuration State Functions (CSFs)

$$\Psi(PJM) = \sum_r c_r \psi_r(PJM) \quad (1)$$

where the label (PJM) states that the linear combination is formed from the CSFs with the same parity P , same total angular momentum J , and one of its projections M . The coefficients c_r describe the mixing of the corresponding CSFs at the ASF, and they represent the electron correlation. Numerical calculations were performed by applying the GRASP92 code^[15] together with the RELCI (relativistic configuration interaction calculation) extension^[16].

The photoionization cross sections from the initial state $(P_i J_i M_i)$ to the final state $(P_f J_f M_f)$ can be written as^[17]

$$\sigma_{if}^{\text{PI}} = 4\pi^2 a_0^2 \alpha \frac{df_{if}}{d\epsilon} \quad (2)$$

where α is the fine structure constant and a_0 is the Bohr radius. Numerical calculations of Eq. (2) were performed using Relphoto08^[14,18-19]. $df_{if}/d\epsilon$ refers to the oscillator strength density, and further details are available in Refs.[14, 18]. In the present work, the final state is the ionic one-hole state that is coupled to the continuum photoelectron to yield the opposite parity as the initial neutral atomic state.

The 2p photoionization of excited states $2p^6 3p_{1/2,3/2}$ of sodium atoms, which gives rise to the $2p^5 4p$ monopole shake-up satellite states, can be written as

$$2p^6 3p(^2P_{1/2,3/2}) + h\nu \rightarrow 2p^5 4p(^1S_0, ^1P_1, ^1D_2; ^3S_1, ^3P_{0,1,2}, ^3D_{1,2,3}) + \epsilon k (l=0, 2) \quad (3)$$

where the photoelectrons are assumed to escape by means of the partial waves $|\epsilon k\rangle$ and with kinetic energies ϵ . The energy $\epsilon = E_i + h\nu - E_f$ is determined by the photon energy $h\nu$ and the total energies of the atom in the initial and final states. The “photoion+electron” system then gives rise to the total final state $|\alpha_f^{N-1}(J_f' P_f' M_f'), \epsilon k; \alpha_f^N(J_f P_f M_f)\rangle$ with total energy $E_f = E_i + h\nu$ after the photon has been absorbed by the atom^[14]. Here, we utilize the relativistic angular-momentum quantum number

$$k = \pm(j + 1/2) \text{ for } l = j \pm 1/2 \quad (4)$$

to denote the symmetry properties of the outgoing photoelectron, i. e., its angular momentum j and parity $(-1)^{l(20)}$.

From the shake theory^[9], the corresponding transition matrix element is $\langle 2p | \hat{o} | \epsilon l \rangle \langle 3p | 4p \rangle$, the first term describes single photoionization in which the orbital of the 2p electron remains unchanged, and the second term accounts for the satellite excitation^[11]. To estimate the shake-up cross sections, several overlap integrals between the initial- and final-state orbitals of the outermost electrons have been calculated. Therefore, the branching ratio between the satellite and main line is thus equal to $|\langle 3p | 4p \rangle|^2 / |\langle 3p | 3p \rangle|^2$. Shake-up satellites arise in the sudden approximation, in which the photoionization causes a sudden change in the Coulomb attraction, and the excited electron changes its orbital quantum number, which implies an exchange of angular momentum between the residual ionic core and the outgoing photoelectron. To compare the results of our calculations with experimental results, the theoretical spectra were convolved with a Gaussian function with a constant energy value to account for the finite experimental resolution.

The most standard approach is to use the active space method. A single or minimal set of reference CSFs serve as a zeroth order basis, and by extending the configuration space stepwise to the limit where reasonable agreement with the experiment was obtained. For a better understanding of electron correlation, a comparison was performed between the single-configuration and multiconfiguration calculations. But it should be pointed out that the spectra structures can be predicted considerably better by multiconfiguration expansion than by single-configuration approximation because prominent electron correlation can be taken into account in the larger configuration set, so the discussion below is based mainly on multiconfiguration calculations. In the calculation of neutral-state wavefunctions, the configurations $1s^2(2s^2 2p^6 3p + 2s^2 2p^6 4p + 2s 2p^6 3s 3p + 2s^2 2p^5 3p^2 + 2s 2p^6 3s 4p)$ were included. To reduce shifting of the average energy, the calculations were performed in two steps. In the first step, the wavefunctions of the sodium atoms were computed in a single configuration approximation, and in the second step, the wavefunctions of the Be-like core were fixed and the outer orbitals were generated. The single ionized state $2p^5 3p$ was computed in a similar way by including the configurations $1s^2(2s^2 2p^5 3p + 2s^2 2p^5 4p + 2s^2 2p^6 + 2s 2p^6 3s + 2s 2p^6 3d)$. For the final states $2p^5 4p$ of the shake-up process, the configurations used were $1s^2(2s^2 2p^5 3p + 2s^2 2p^5 4p + 2s^2 2p^5 4f + 2s^2 2p^6 + 2s 2p^6 3s + 2s 2p^6 3d)$ in the second step. In this case, the final-core wavefunctions were obtained from the single configuration calculation, and all outer orbitals were set to be free in a multiconfiguration iteration.

2 Results and discussions

For the single photoionization $2p^6 3p \rightarrow 2p^5 3p(^1S_0, ^1P_1, ^1D_2; ^3S_1, ^3P_{0,1,2}, ^3D_{1,2,3})$, 10 fine-structure energy levels were constructed from the final ionic configuration $2p^5 3p$, as well as from the configuration $2p^5 4p$ of the $2p^6 3p \rightarrow 2p^5 4p$ shake-up process. From the NIST database^[21] or our present calculations, for the final configuration $2p^5 3p$, the ascending energy order is $^3S_1, ^3D_3, ^3D_2, ^3D_1, ^1D_2, ^1P_1, ^3P_2, ^3P_0, ^3P_1$ and 1S_0 , which are denoted by labels 1~10 in Figs.1 and 2, as shown in the following discussion. For example, the peaks labelled as 3 and 5 denote states 3D_2 and 1D_2 arising from the photoionization $2p^6 3p \rightarrow 2p^5 3p$, respectively.

To explore the influence of electron correlation effects on the spectra structure, we performed calculations within both the single configuration approximation and multiconfiguration approximation that accounts for more electron correlations in Eq. (2). The 2p photoelectron spectra arising from the single photoionization $2p^6 3p$

($^2P_{1/2}$) $\rightarrow 2p^53p$ of sodium atoms at the photon energy $h\nu=54$ eV are presented in Fig.1. The solid (red dash) line in the right panel, which was generated with experimental energy resolution assuming a Gaussian instrument function, is the spectrum simulated with wavefunctions from the multiconfiguration (single) approximation. The vertical lines in the right panel indicate the calculated intensities and energy positions of the photolines with wavefunctions from the multiconfiguration approximation. As shown, the agreement of the simulated spectrum compared to the experimental one presented in the left panel is good^[22]; in particular, the middle parts of the spectrum are well reproduced. For comparison, the calculated spectra are normalized to the dominant intensity of final ionic state $2p^53p(^3D_2)$, and the calculated energies are shifted by +1.51 eV to coincide with the experiment. The peaks were identified by comparing the experimental spectrum to the present MCDF calculations.

As shown in Fig.1, the spectrum lines are separated into singlets and triplets, which are typical for LS-coupled systems, whereas the energy ordering of the lines deviates from Hund's rules. This deviation can be explained by the non-negligible spin-orbit interaction of the electrons. Our MCDF energy calculations in the *jj*-coupled basis show that peaks 1~6 arise from the $2p_{3/2}$ hole final states $2p^53p(^3S_1, ^3D_3, ^3D_2, ^3D_1, ^1D_2, ^1P_1)$, whereas peaks 7~10 correspond to final states $2p^53p(^3P_2, ^3P_0, ^3P_1, ^1S_0)$ having a hole in the $2p_{1/2}$ orbital. As expected, the contribution of electron correlation leads to a significant shift in the relative energy position, particularly for states 3S_1 and 1S_0 , which are labelled as 1 and 10 in the figure, but it is not the same case for intensities.

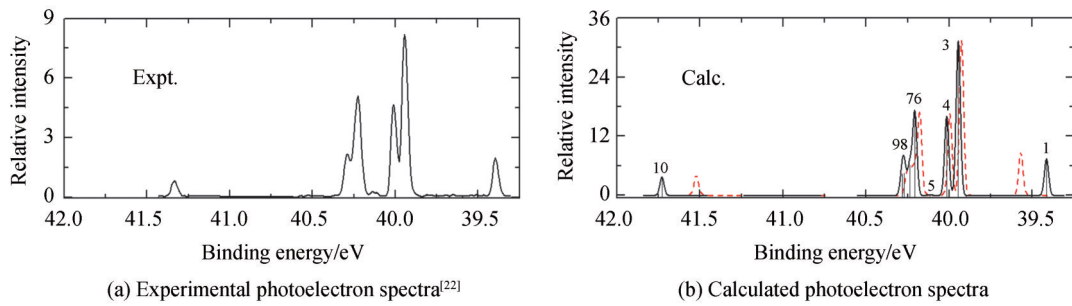


Fig.1 $2p$ photoelectron spectra arising from the single photoionization of initial state $2p^63p(^2P_{1/2})$

For sodium atoms, spin-orbit coupling is so strong that the $3p_{1/2}$ and $3p_{3/2}$ orbitals can be separated. According to the NIST database^[21] or the present calculations, the difference of the 10 fine-structure energy levels is 0.002 eV. To elucidate the influence of spin-orbit effects, the photoelectron spectra of sodium atoms from the initial excited $2p^63p(^2P_{3/2})$ are shown in Fig.2. Of course, the solid (red dash) line in the right panel is the spectrum from the multiconfiguration (single) approximation, but the calculated spectra are normalized to the intensity of the final ionic state $2p^53p(^3D_3)$. A similar theoretical analysis can be applied to this case. As shown, the spectrum structures are predicted by the calculations very well, even when the calculated spectra are shifted +1.51 eV to higher energies compared to the experimental results^[23]. This shift is primarily caused by electron correlation; again, the peaks from the final states 3S_1 and 1S_0 are found to be very sensitive to the configuration basis used in the calculations.

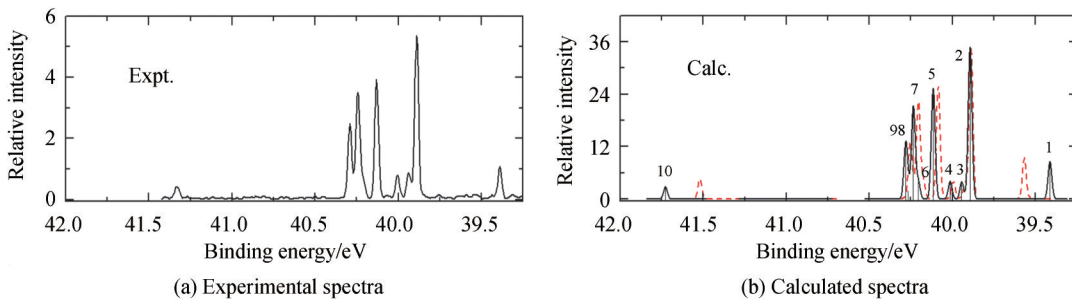


Fig.2 Same as Fig.1 but for the photoionization of initial state $2p^63p(^2P_{3/2})$

More importantly, it is well known that relativistic effects play only a fairly small role in low- Z elements. However, the present results show that the relativistic effects are strong for the spectra structure from the 2p inner-shell photoionization of sodium atoms. Comparison of Figs 1 and 2 indicates that the total angular momentum J of the initial state $2p^63p(^2P_{1/2,3/2})$ has an obvious influence on the photoelectron spectra, whereas the structures clearly resemble each other. This result is not surprising because for 2p photoionization from excited states $2p^63p(^2P_{1/2,3/2})$, there are two open subshells, and special care must be taken to construct the wavefunctions.

The spectra obtained from $2p^63p(^2P_{1/2,3/2}) \rightarrow 2p^54p(^1S_0, ^1P_1, ^1D_2; ^3S_1, ^3P_{0,1,2}, ^3D_{1,2,3})$ shake-up transitions at a photon energy of $h\nu=48$ eV are shown in Figs. 3 and 4. Then, the labels refer to the peaks for the ten final ionic states $2p^54p$, the calculated spectra are normalized to the intensity of the final ionic state $2p^53p(^3D_2)$ in Fig.3 but $2p^53p(^3D_3)$ in Fig.4. As clearly shown, our current calculations including full relaxation appear to provide fairly reasonable results. By comparing the experimental and simulated satellite structures from the single configuration approximation, it can be observed that the agreement is considerably worse than for the main spectra. For example, the calculated spectra are shifted by $+3.75$ eV to coincide with the experiment^[12], and some intensities are overestimated while others are underestimated, such as the leftmost intensities of the final ionic state $2p^54p(^1S_0)$ in the figures. The large shift may follow partially from the uncertain factors, which depend on the geometry of the reaction volume. Subsequently, the other part most likely follows from the 4p wavefunction because the single configuration, and even the multiconfiguration approximation, was not able to produce the 4p radial wavefunction correctly. However, these results indicate that the energy splitting of the intensities is more difficult to calculate correctly, but more importantly, the satellites are caused by electron-electron interactions, which obviously makes the intensity calculations more difficult and sensitive to the correctness of the wavefunctions.

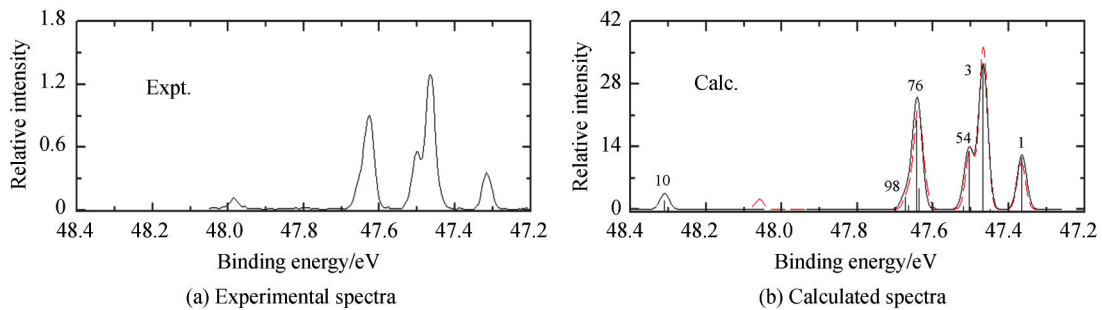


Fig.3 Same as Fig.1 but for the $2p^63p(^2P_{1/2}) \rightarrow 2p^54p$ shake-up satellites

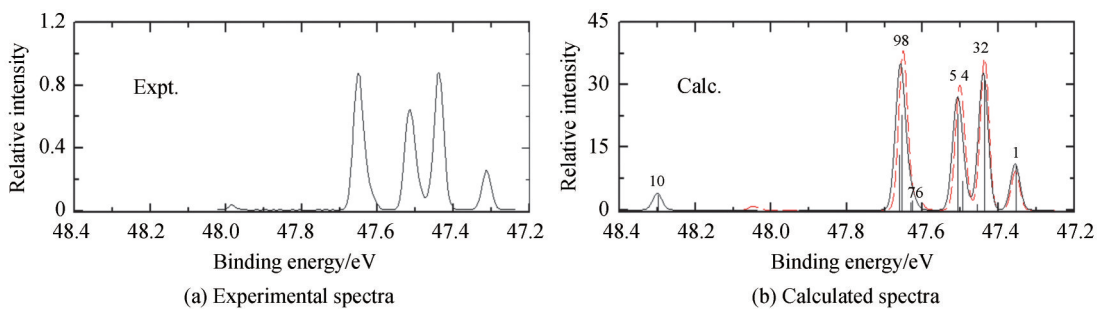


Fig.4 Same as Fig.3 but for the $2p^63p(^2P_{3/2}) \rightarrow 2p^54p$ shake-up satellites

As expected, the satellite spectrum shows that the spacing of energy levels decreases compared to the $2p^63p \rightarrow 2p^53p$ spectrum. The total width of the satellite spectrum is less than 1 eV, whereas that of the main spectrum is greater than 2 eV. The decrease in the energy spacing originates from the coupling change of the outermost electron, even though the jj coupled terms are completely the same in the two cases. For final configuration $2p^54p$, the ascending energy order is $^3S_1, ^3D_3, ^3D_2, ^1P_1, ^3P_2, ^3P_0, ^3D_1, ^1D_2, ^3P_1$ and 1S_0 , which are denoted by labels 1~10 in Figs. 3 and 4, i. e., the energy order is adjusted compared to $2p^53p$ and the singlet-triplet

structure is obviously broken. The peaks corresponding to the final states $2p^54p(^3S_1, ^3D_3, ^3D_2)$ are still at the three lowest binding energies, and $2p^54p(^3P_1, ^1S_0)$ are the two highest binding energies. The appearance of the *jj* coupled feature in the satellite spectra in Figs.3 and 4 shows that the spin-orbit interactions are more important in $2p^63p(^2P_{3/2}) \rightarrow 2p^54p$ shake-up transitions. It can be observed that the difference between the main and satellite spectra is significant, which means that the main spectrum structures divided by the coupling of $2p^{-1}$ holes also appear in the satellite spectra, but some of the structures are modified due to the changes in coupling of the outermost electron and mixing of configurations. In addition, the results demonstrate the sensitivity of satellite spectra to probe electron correlation in shake-up transitions and suggest that despite the large size of multiconfiguration expansion, the basis is still not sufficient to correctly account for the electron correlation.

To more clearly illustrate the influence of the incident photon energy on the satellite spectrum, the spectra calculated with wavefunctions from the multiconfiguration approximation for different incident photon energies are shown in Fig.5. The solid lines are the calculated results for a photon energy of $h\nu=54$ eV, and the (red) dash lines are for $h\nu=48$ eV. As shown in this figure, the calculations performed for the two photon energies yield virtually identical photoelectron spectra, whereas the differences between the leftmost intensities of the final ionic state $2p^54p(^1S_0)$ cannot be regarded as negligible. This behaviour follows from the fact that while at different photon energies, the satellite photoelectron structures are mainly determined by the target atoms and the relative intensities of the photolines may not show any photon energy dependence over a certain energy range, as clearly emphasized in Ref. [12], even though the shake-up process is generally believed to be sensitive to the incident photon energy.

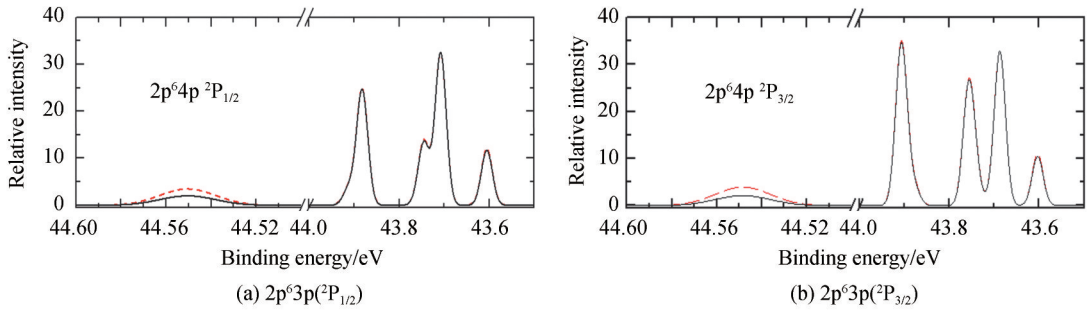


Fig.5 Theoretical 2p photoelectron spectra arising from the $2p^63p(^2P_{1/2,3/2}) \rightarrow 2p^54p$ shake-up transitions

To explore the main and shake-up processes with a unified standard and to obtain a deeper physical understanding, the 2p photoelectron spectra calculated with wavefunctions from the multiconfiguration approximation at a photon energy of $h\nu=54$ eV are shown in Fig.6. The solid lines are the main spectra arising from the $2p^63p \rightarrow 2p^53p$ photoionization of sodium atoms, and the (red) dashed lines are the satellite spectra from the $2p^63p \rightarrow 2p^54p$ shake-up transitions. Again, the spectra from the initial state $2p^63p(^2P_{1/2})$ in the left panel are normalized to the intensity of the final ionic state $2p^53p(^3D_2)$, and the spectra from the initial state $2p^63p(^2P_{3/2})$ in the right panel are normalized to the intensity of $2p^53p(^3D_3)$. For the main spectrum from initial state $2p^63p(^2P_{1/2})$, the intensity of the final state $2p^53p(^3D_2)$ is the highest. However, in the case of $2p^63p(^2P_{3/2})$, the intensity of the final state $2p^53p(^3D_3)$ becomes the highest. Therefore, the spectra from the initial state $2p^63p(^2P_{1/2})$ are normalized to the dominant intensity of the final ionic state $2p^53p(^3D_2)$, and the spectra from the initial state $2p^63p(^2P_{3/2})$ are normalized to the intensity of $2p^53p(^3D_3)$. As discussed above, these satellites primarily arise from the rearrangement of electron density during the course of photoionization, which gives rise to a finite shake-up probability for the 3p valence electron. By comparing the main and satellite spectra in Fig. 6, one can observe that the overall intensities of the $2p^63p \rightarrow 2p^54p$ shake-up transitions are smaller compared to the $2p^63p \rightarrow 2p^53p$ photoionization, i. e., shake-up transitions are weak compared to normal photoionization transitions, as generally expected^[13,24]. This result is due to the smaller overlap between the initial-and final-state orbitals of the outermost 3p and 4p electrons, as described $\langle 2p | \hat{o} | \epsilon l \rangle \langle 3p | 4p \rangle$, respectively.

However, as shown in Fig. 6, the relative intensities of the shake-up transitions are quite obvious compared to the main spectra. According to the present calculations, some shake-up intensities are found to be

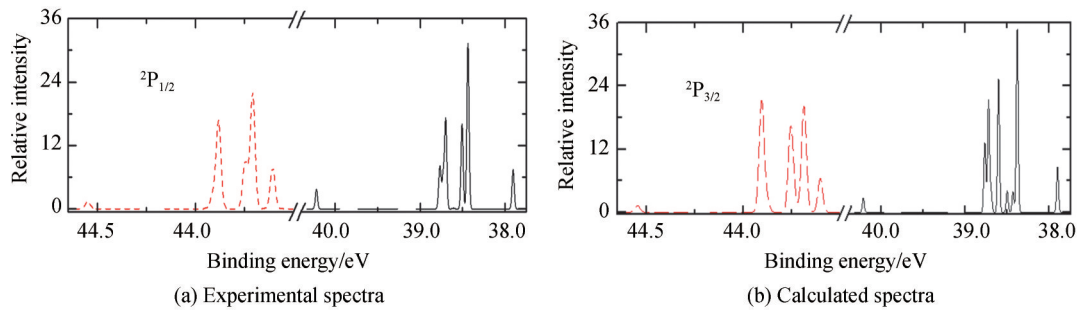


Fig.6 Theoretical 2p main and satellite photoelectron spectra of sodium atoms

more than 50% of the corresponding main transitions. This result tends to indicate a strong orbital relaxation because of the removal of a 2p electron and the importance of shake-up processes in the case of sodium. The physical model used for the monopole shake-up transition is a simultaneous dipole transition and an electron excitation into the higher orbital. In this simple picture, these originate exclusively from the substantially larger overlap $\langle 3p|4p \rangle$ between neutral 3p and ionic 4p radial wavefunctions. The present calculations show that the atomic 3p mean orbital radius is $5.99a_0$, the ionic 4p mean orbital radius is $8.02a_0$, and the 3p mean orbital radius is $3.71a_0$. Note that the orbital relaxation may lead to an increase in the overlap between neutral 3p and ionic 4p radial wavefunctions compared to the overlap $\langle 3p|3p \rangle$ between neutral and ionic 3p radial wavefunctions, i.e., to an increase in the satellite intensities compared to the main ones, even though the single photoionization is still the strongest process.

3 Conclusion

The 2p photoelectron spectra of sodium atoms from the initial states $2p^63p(^2P_{1/2,3/2})$ and the satellite spectra originating from the corresponding shake-up transitions during the 2p photoionization have been investigated using MCDF method. In our theoretical analysis, special emphasis was placed on the influence of electron correlation on the photoelectron spectra. It has been shown that the theoretically predicted photoelectron spectrum is in good agreement with the experimental results, allowing us to identify the photolines.

It is also shown that the spin-orbit effects have an important role in forming the photoelectron spectra. As expected, the main photoelectron spectrum spans a considerably broader energy region than the $2p^63p \rightarrow 2p^54p$ satellite spectrum, and the shake-up transitions are weak compared to the normal transitions. However, the relative intensities of shake-up transitions are very obvious compared to the main spectra. The reason is the strong relaxation effects due to the collapse of 3p orbital after the emission of 2p photoelectron, which leads to an increase in the shake-up intensities.

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