CHIN. PHYS. LETT. Vol. 38, No. 5 (2021) 053201

Core-Excited Molecules by Resonant Intense X-Ray Pulses Involving Electron-Rotation Coupling

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(Received 26 January 2021; accepted 9 March 2021; published online 2 May 2021)

It has been reported that electron-rotation coupling plays a significant role in diatomic nuclear dynamics induced by intense VUV pulses [Phys. Rev. A 102 (2020) 033114; Phys. Rev. Res. 2 (2020) 043348]. As a further step, we present here investigations of the electron-rotation coupling effect in the presence of Auger decay channel for core-excited molecules, based on theoretical modeling of the total electron yield (TEY), resonant Auger scattering (RAS) and x-ray absorption spectra (XAS) for two showcases of CO and CH^+ molecules excited by resonant intense x-ray pulses. The Wigner D-functions and the universal transition dipole operators are introduced to include the electron-rotation coupling for the core-excitation process. It is shown that with the pulse intensity up to 10^{16} W/cm^2, no sufficient influence of the electron-rotation coupling on the TEY and RAS spectra can be observed. This can be explained by a suppression of the induced electron-rotation dynamics due to the fast Auger decay channel, which does not allow for effective Rabi cycling even at extreme field intensities, contrary to transitions in optical or VUV range. For the case of XAS, however, relative errors of about 10% and 30% are observed for the case of CO and CH^+, respectively, when the electron-rotation coupling is neglected. It is concluded that conventional treatment of the photoexcitation, neglecting the electron-rotation coupling, can be safely and efficiently employed to study dynamics at the x-ray transitions by means of electron emission spectroscopy, yet the approximation breaks down for nonlinear processes as stimulated emission, especially for systems with light atoms.

DOI: 10.1088/0256-307X/38/5/053201

In the past few decades, the advent and rapid development of the x-ray free-electron laser (XFEL) facilities[1−5] have made it possible to study target-specific localized inner-shell electrons or holes dynamics in atoms, molecules and materials, by x-ray absorption spectrum (XAS) and resonant Auger scattering (RAS) spectroscopy[6−8] for dynamics on femtosecond and even attosecond timescales.[9−12] Conventional RAS have become a well established tool in x-ray region to investigate the inner-shell electron excitation dynamics in atoms and molecules.[13−16] With the tremendously increased x-ray pulse intensities that are available from modern XFEL facilities, many physical processes and effects that are not visible in weak field have started to play an important role. Multiple Rabi cycles,[17] direct photoionization,[18] Auger spectral broadening,[19] two photon excitation,[20] multi-photon multiple ionization and dissociation,[21−26] and so on, should be taken into account to simulate correctly the XAS and RAS spectra in the intense XFEL radiation.

Recently, it has been shown that the electron-rotation coupling could play a significant role in diatomic rotational dynamics induced by intense VUV pulses on valence electron excitation transitions,[27,28] which was conventionally neglected in most of the theoretical models used so far for prediction of the photoexcitation and photodissociation dynamics.[29−34] This approximation is usually valid in the weak-field conditions since the mass of electron is more than three orders of magnitude smaller than that of nucleus.[35−37] However, the validity of neglecting the electron-rotation coupling in the strong laser pulse condition needs to be examined carefully.[27,28] Given that the XFELs' intense x-ray pulse is now widely available, it has become quite important to reveal the effects of electron-rotation coupling by intense x-ray pulses for core-excited diatomic molecules. Here, we

Supported by the National Natural Science Foundation of China (Grant Nos. 11934004, 11974230, and 11904192), and the Education of Russian Federation (Grant No. FSRZ-2020-0008).
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examine the coupling effect in XAS and RAS spectra, reflecting directly the core-excited wave-packet dynamics[6−8,38] for the showcases of the CO and CH^+, and we compare the results obtained with and without electron-rotation coupling included. In our simulations, we suppose XFEL pulse duration comparable to the Auger decay lifetime at the carbon K-edge of the CO or CH^+ $\tau_d \approx 8.2$ fs.[39] Since the reduced mass of CH^+ is about seven times smaller than that of CO, it results in a much faster rotational and vibrational dynamics. Thus, rather different effects of the electron-rotation coupling on CO and CH^+ are expected. Our analysis shows that there is no visible effect related to the electron-rotation coupling on the total electron yield (TEY), molecular population of ground state and RAS spectra, while for molecular alignment of the ground state and XAS at high fields intensities show an effect of about 30% for the case of the lighter CH^+ molecule, and about 10% for CO. The diminishing of the effect is explained by the presence of the fast Auger decay dissipative channel. Consequently, the electron-rotation coupling contribution can be safely neglected in calculations of the electron emission spectra on the x-ray transition, especially with the lifetime of the core-excited state shorter than that of C K-edge studied here.

This work theoretically studies the effect of electron-rotation coupling on the dynamics in molecules excited in the x-ray region in the presence of the Auger decay channels and is organized as follows. First, the theoretical framework is briefly outlined, then followed by discussions of numerical results. Finally, a conclusion is given. Unless otherwise stated, atomic units ($e = m_e = \hbar = 1$) are used throughout.

Theoretical Methods. Our theoretical approach is based on the time-dependent wave-packet propagation method.[19,38,40] Here, it is applied to study of the nuclear dynamics triggered by a linearly polarized resonant x-ray pulse with polarization vector orienting along Z axis in the space-fixed (SF) framework. Our calculation involves the transitions between the initial (ground) electronic state Φ_I, the core-excited (resonant) electronic state Φ_R, and the final electronic state of the Auger decay process Φ_A^ε (single ionized molecule with an electron of energy ε), with the nuclear wave-packets $\Psi_I(t)$, $\Psi_R(t)$, and $\Psi_A(\varepsilon, t)$, respectively. Within the rotating wave approximation[41−43] and the local approximation,[44−47] the rovibronic working equation for a specific final Auger state with electron free energy ε is given as[19,38,40]

$$i\frac{\partial}{\partial t}\Psi(\varepsilon,t) = \hat{H}(q,\varepsilon,t)\Psi(\varepsilon,t), \tag{1}$$

where $\Psi(\varepsilon,t) = [\Psi_I(t)\Psi_R(t)\Psi_A(\varepsilon,t)]^T$, and

$$\hat{H}(q,\varepsilon,t) = -\frac{1}{2\mu}\frac{\partial^2}{\partial q^2} + \frac{\boldsymbol{R}^2}{2\mu q^2} + \begin{pmatrix} V_I(q) & D^\dagger(t)\kappa^\dagger(\beta,\gamma) & 0 \\ D(t)\kappa(\beta,\gamma) & V_R(q) - \dfrac{i\Gamma_{\rm Aug}}{2} - \omega & 0 \\ 0 & V & V_A(q) + \varepsilon - \omega \end{pmatrix}. \tag{2}$$

The Hamiltonian $H(q,\varepsilon,t)$ is a physical quantity relating to the nuclear distance q, the Auger electron energy ε, and the time t; μ is the reduced mass and ω is the frequency of excitation light. The first and second terms on the right-hand side of Eq. (2) represent the vibrational and rotational kinetic energy operators, respectively. The rotational angular momentum of the molecule $\boldsymbol{R}$ satisfies $\boldsymbol{R}^2 = \boldsymbol{J}^2 - \Omega^2$, where $\boldsymbol{J} = \boldsymbol{R} + \Omega\hat{\boldsymbol{z}}$ is the molecular total angular momentum and Ω is the projection of the total electron internal angular momentum on the molecular-fixed (MF) z axis (molecular axis). Note that $\boldsymbol{R}$ and Ω are intrinsically coupled in Hund's case (a); $V_I(q)$, $V_R(q)$, $V_A(q)$ are the potential energy curves of the corresponding electronic states (see Fig. 1); $D(t) = d_{IR}g_0g_t/2$ is the dipole interaction with the dipole transition element $d_{IR} = \langle\Phi_R|\hat{r}|\Phi_I\rangle$, the electric field peak intensity g_0, and the electric field envelope g_t; the Auger decay width $\Gamma_{\rm Aug} = 2\pi|V|^2$, which is 0.08 eV for carbon core-excited states of CO and CH^+ (about 8.2 fs). In conventional treatment (neglecting electron-rotation coupling or setting $\Omega = 0$), $\kappa(\beta,\gamma) = \sin\beta$, and Legendre polynomials or spherical harmonics are used to describe the rotational dynamics. As revealed in our previous works,[27,28] in a more general approach, which includes the intrinsic coupling between $\boldsymbol{R}$ and Ω ($\boldsymbol{R}$–Ω coupling), the value $\kappa(\beta,\gamma) = \sin\beta e^{i\gamma}$ for the transition between Σ and Π states, and the angular functions should be expressed using L_2-normalized Wigner D-functions $|JM\Omega\rangle = (\frac{2J+1}{8\pi^2})^{\frac{1}{2}} D^J_{M,\Omega}(\alpha,\beta,\gamma)$, where $D^J_{M,\Omega}(\alpha,\beta,\gamma)$ is the Wigner D-function,[27] M is the projection of $\boldsymbol{J}$ onto the SF Z axis (laser polarization), α, β and γ represent the Euler angles between SF and MF axes. Explicitly, β is the angle between laser polarization and the molecular axis.

The RAS spectrum can be computed as a norm of final ionic wave-packet $\Psi_A(\varepsilon,t)$ at long time given as[19,46,48]

$$\sigma_A(\varepsilon) = \lim_{t\to\infty}\langle\Psi_A(\varepsilon,t)|\Psi_A(\varepsilon,t)\rangle. \tag{3}$$

The molecular XAS spectrum $S(\omega)$ can be expressed as[38]

$$S(\omega) = -2\mathrm{Im}[\mu(\omega)E^*(\omega)]. \tag{4}$$

Here $\mu(\omega)$ and $E(\omega)$ are the Fourier transforms of the time-dependent induced dipole $\mu(t) = \langle\Psi(t)|\hat{\mu}|\Psi(t)\rangle$ and the electric field $E(t)$ of the light pulse, respectively. The Gaussian envelope $g(t) = g_0 e^{-(t-t_0)^2/\tau^2}$ is employed in the calculation with $\tau = 10$ fs, g_0 is the electric field peak intensity. The ground state time-dependent population $P_{\rm I}(t)$, the total electron yield $P_{\rm T}^{\varepsilon}$, and the molecular alignment $\langle\cos^2\rangle_{\rm I}(t)$ can be computed by

$$\begin{aligned} &P_{\rm I}(t) = \langle\Psi_{\rm I}(t)|\Psi_{\rm I}(t)\rangle, \\ &P_{\rm T}^{\varepsilon} = \int d\varepsilon\sigma_{\rm A}(\varepsilon) = 1 - P_{\rm I}(t\to\infty), \\ &\langle\cos^2\rangle_{\rm I}(t) = \frac{\langle\Psi_{\rm I}(t)|\cos^2\beta|\Psi_{\rm I}(t)\rangle}{P_{\rm I}(t)}. \end{aligned} \tag{5}$$

In the present model, the direct photo-electron emission is neglected and only the Auger decay channel yields free electrons, which allows to clearly present the effect of $\boldsymbol{R}$–Ω coupling.

Next, we discuss the numerical quantities, such as electron yield, population, alignment, RAS and XAS spectra, for CO and CH^+ computed by the conventional and refined theoretical treatments, without and with $\boldsymbol{R}$–Ω coupling included, respectively. All the potential energy curves of CO are described by Morse potentials with parameters from Ref. [49]. Morse potentials for the ground and final ionic states of CH^+ are from Refs. [50,51], while the potential energy curve of the core-excited state was obtained by fitting the experimental data.[29] The pump pulse is tuned at $\omega = 287.4$ eV and $\omega = 286.84$ eV for CO and CH^+, respectively, for resonant excitation from the ground to the lowest carbon 1s core-excited state[38,29] (see Fig. 1).

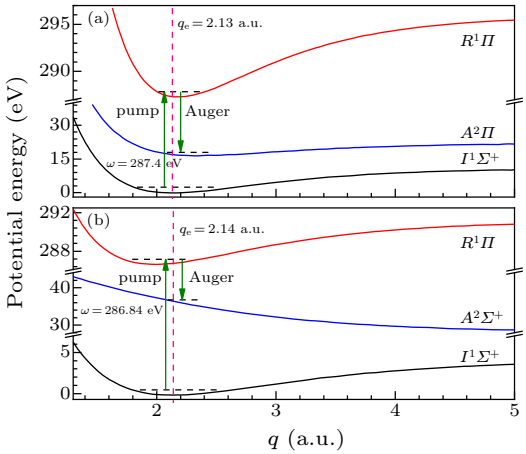

Fig. 1. Potential energy curves for the three involved electronic states in CO (a) and CH^+ (b). The molecules are resonantly pumped by intense x-ray pulse from the ground state $I^1\Sigma^+$ to the core-excited state $R^1\Pi$, accompanied by Auger decay to the bound (CO) and dissociative (CH^+) ionic states. The ground state equilibrium distance is marked by the dashed pink line.

To solve the rovibronic working equation, the radial part of the nuclear wave function is expanded by 91 (161) sin-DVR basis functions for CO (CH^+) in the range of [1.7,4.7] ([0.5,12.0]). A complex absorbing potential (CAP) $-iW(q) = -i\eta(q-q_c)^3\Theta(q-q_c)$ with starting point $q_c = 6$ a.u. and strength $\eta = 0.005$ a.u. was added to the final ionic dissociative state of CH^+ to calculate its RAS spectra through flux analysis, Θ is Heaviside's step function. For the rotational degree of freedom, β was expanded by 51 Legendre polynomial basis functions in the conventional treatment; and 51 Wigner basis functions for β, 7 exp-DVR basis functions for γ and 1 k-DVR basis function for α were used in the improved theoretical framework.[27,28] The Heidelberg multiconfiguration time-dependent Hartree (MCTDH) package is implemented for the calculations.[40,52]

Results and Discussion. The total electron yield as a function of x-ray pulse intensity, defined in terms of Rabi frequency $\Omega_{\rm Rabi} = d_{\rm IR}g_0$ for CO molecule, with and without $\boldsymbol{R}$–Ω coupling, is depicted in Fig. 2 (a), which shows an increasing yield to about 80% accompanied by weak and smoothed Rabi oscillations. The effect of $\boldsymbol{R}$–Ω coupling is negligible, the difference in the whole intensity range is within 0.1%, even with $\Omega_{\rm Rabi}$ up to 1.5 eV (corresponding to six Rabi cycles, or peak intensity about 10^{16} W/cm^2). Let us now look at the time-dependent population and molecular alignment in the ground state, and XAS for $\Omega_{\rm Rabi} = 1.5$ eV presented in Figs. 2(b)–2(d), respectively. It can be seen that the Rabi flopping is also imprinted in the time-dependent ground state population, computed in both models, as well as in the difference between them (error of neglecting of the $\boldsymbol{R}$–Ω coupling, see the blue curve). The error increases in time yet stays very tiny within 0.1% [Fig. 2(b)]. Field-free molecular alignment in the ground state created by the strong x-ray pulse shows a periodical dynamics with an error value increased up to about 10% [Fig. 2(c)]. Molecular alignment is an observable directly related to the molecular rotation,[27,28] so much larger effect of electron-rotation coupling is not surprising. Let us now discuss XAS [see Fig. 2(d)], which reflects the wave-packet dynamics on the both ground and core-excited states, coupled by the strong x-ray pulse [see Eq. (4)]. The structure of the XAS profile shows that the main absorption peak is around 287.4 eV (the resonant excitation energy between the ground state $|v=0\rangle_{\rm I}$ and the core-excited state $|v=0\rangle_{\rm R}$), along with a negative side peak (emission), which is an important characteristic of the interaction with the intense field.[38] It is interesting to note that the $\boldsymbol{R}$–Ω coupling effect in XAS has the value of about 10%, similar to the case of the molecular alignment [Fig. 2(c)], even though the x-ray absorption is not an observable concerned directly to the molecular

rotation.

The main difference of the photo-induced transition in x-ray region, from the VUV-pump on the valence transitions[27,28] is the presence of the additional fast Auger process, which decreases dramatically the lifetime of the excited state by the nonradiative decay channels. Due to this, all induced dynamics of the excited ro-vibrational wave-packet is developed within rather short Auger lifetime, resulting in much weaker effect of the $\boldsymbol{R}$–Ω coupling for the x-ray range, contrary to VUV excitation. This is the main reason for suppression of electron-rotation coupling influence in the above discussed case of CO molecule, excited on C K-edge. In general, the excited ro-vibrational wave-packet has much more significant dynamics for the lighter systems, having shorter rotational and vibrational periods, even the Auger lifetime of the core-excited state is the same. Specifically, we considered here CH^+, with reduced mass about seven times smaller as compared to CO, yet excited on the same C K-edge. According to the above discussion, one can expect more significant dynamics induced by $\boldsymbol{R}$–Ω coupling effect.

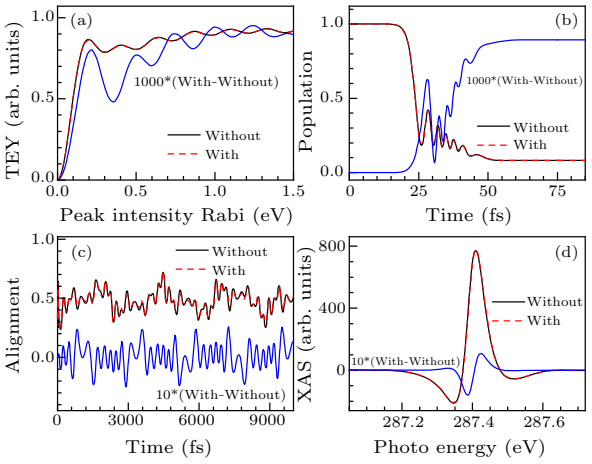

Fig. 2. Total electron yield (TEY) as a function of the Rabi frequency $\Omega_{\rm Rabi}$ (a); time evolution of the population (b) and molecular alignment (c) in the ground state; XAS spectra (d). Simulations are performed for CO molecule excited by 10 fs resonant intense x-ray pulses, $\Omega_{\rm Rabi} = 1.5$ eV (b)–(d). Solid-black and dashed-red lines represent the calculations without and with $\boldsymbol{R}$–Ω coupling included, respectively; the difference between the two approaches (error) is shown by solid blue lines.

The results of our simulation for the case of CH^+ resonantly pumped by intense x-ray pulse at $\omega = 286.84$ eV (from the ground $|v = 0\rangle_{\rm I}$ to the core-excited $|v = 0\rangle_{\rm R}$ vibrational levels) are presented in Fig. 3 (the figure is organized exactly as Fig. 2 for easier comparison). The figure clearly shows that the difference from $\boldsymbol{R}$–Ω coupling increases to about 0.5% for the TEY spectra [Fig. 3(a)] and time-dependent population of the ground state [Figs. 3(b)]. The most dramatic effect appears in the alignment of the ground state, which is an error of about 30% due to neglecting the $\boldsymbol{R}$–Ω coupling [Figs. 3(c)] and XAS [Figs. 3(d)]. As discussed above, the rather strong effect of the electron-rotation coupling in the case of molecular alignment is not surprising given that the observable is directly related to the rotational dynamics. A quite strong effect in XAS can be explained by induced electronic transitions (stimulated emission) in the intense x-ray pulse, which inherently includes the Rabi flopping dynamics. Let us note that XAS have been already effectively implemented[29] in the study of the electronic structures of CH^+.

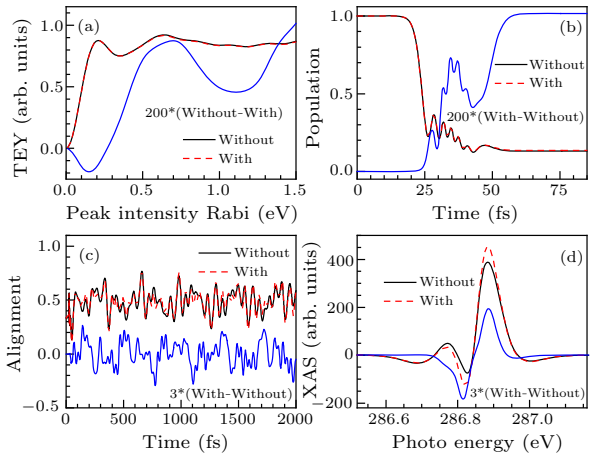

Fig. 3. The same as in Figs. 2 but for the case of CH^+ molecule.

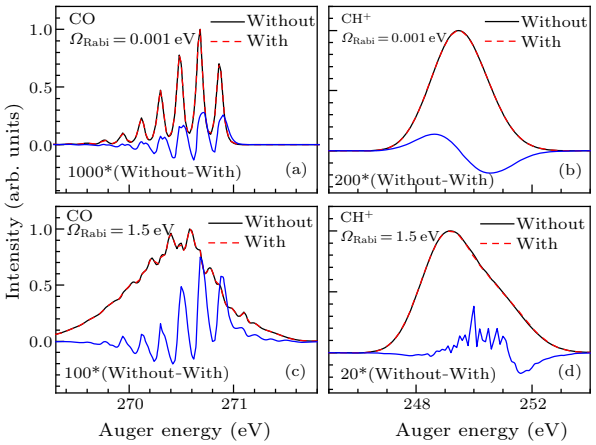

Fig. 4. RAS spectra of CO (left panels) and CH^+ (right panels) molecules excited by 10 fs resonant x-ray pulse calculated with (red-dashed curves) and without (black-solid curves) $\boldsymbol{R}$–Ω coupling, the difference between the two models is shown in blue-solid curves in all panels. The case of the weak $\Omega_{\rm Rabi} = 0.001$ eV (upper panels) and intense 1.5 eV (lower panels) pulses are considered.

The RAS spectra of CO and CH^+ for both weak and strong field with and without $\boldsymbol{R}$–Ω coupling are also investigated and presented in Fig. 4. This figure shows that in the weak field, the vibrational structures of CO are clearly resolved,[38] CH^+ exhibits a quite broad peak due to the dissociative nature of the final

state in CH^{2+}. The effect of $\boldsymbol{R}$–Ω coupling is about 0.1% and 0.5% for CO and CH^+, respectively, consistent with the differences for the TEY and population dynamics simulations [Figs. 2(a) and 2(b), Figs. 3(a) and 3(b)]. In the case of the intense field [Fig. 4(c) and 4(d)], the field broadening of the vibrational peaks smear out the fine structures in CO.[19] Moreover, both the main structure of CO and the peak maximum of CH^+ RAS shift slightly to the lower energy region due to the dressing of the core-excited state by the intense pulse.[20,28] The difference from $\boldsymbol{R}$–Ω coupling in the intense field case ($\Omega_{\rm Rabi} = 1.5\,{\rm eV}$) increases significantly to 1% and 5% for CO and CH^+, respectively. Apparently, the lighter system with shorter rotational period is strongly affected by the $\boldsymbol{R}$–Ω coupling in RAS spectra.

Besides the results presented and discussed above, broader investigations of the $\boldsymbol{R}$–Ω coupling effect by varying the pulse duration and the Auger lifetime broadening have also been performed (not shown here), which confirm our main conclusion that any change of the system allowing for more prolonged rotational dynamics would increase the effect of $\boldsymbol{R}$–Ω coupling. Consequently, a lighter molecule with smaller decay width pumped by a longer intense x-ray pulse would show a stronger effect of the $\boldsymbol{R}$–Ω coupling. However, the core-excited state life time becomes shorter for heavier atoms and the transition dipole moment for the core-electron excitation becomes smaller for deeper cores making smaller the interaction strength, which in principle allows us to safely neglect the $\boldsymbol{R}$–Ω coupling effect for higher x-ray energy range (O K-edge etc.), even for the high pulse intensity (up to $10^{16}\,{\rm W/cm^2}$).

In summary, we have investigated the effect of $\boldsymbol{R}$–Ω coupling in the diatomic systems pumped by ultrashort intense pulses in x-ray region. In contrast to the pump process in VUV region, the additional Auger decay channel is present in the core-excited molecules and competes with the rovibrational dynamics induced by $\boldsymbol{R}$–Ω coupling. The total electron yield, molecular population and alignment of the ground state, XAS and RAS spectra in resonant intense x-ray pulses for showcases CO and CH^+ have been studied theoretically. Our results show a negligibly small effect in TEY, RAS, and population dynamics with the x-ray pulse intensity up to $10^{16}\,{\rm W/cm^2}$. This can be explained by the short lifetime of the core-excited state due to fast Auger decay channels, which quenches rather slow rotational dynamics. At the same time, considerably strong effect of the $\boldsymbol{R}$–Ω coupling is shown for the molecular alignment and XAS, resulting from the nonlinear coupling effects in the strong fields on x-ray transitions. As a general trend, the effect of $\boldsymbol{R}$–Ω coupling becomes more significant for longer x-ray pulses, for the lighter systems, and with smaller Auger decay width. The maximum error by neglecting the $\boldsymbol{R}$–Ω coupling is about 30% for the alignment and XAS spectra for CH^+ with $\Omega_{\rm Rabi} = 1.5\,{\rm eV}$. In principle, the $\boldsymbol{R}$–Ω coupling effect would decrease dramatically for heavier atoms, excited on the K-edge, and the conventional theoretical treatment neglecting electron-rotational coupling can be safely and efficiently employed. However, the coupling may become drastically important for the processes at L-edges of heavier element, where the Auger decay rate is smaller and thus an exact description of the $\boldsymbol{R}$–Ω coupling effect is necessary.

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