Field-free molecular orientation induced by combined femtosecond single- and dual-color laser pulses: The role of delay time and quantum interference*

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The coherent control of field-free molecular orientation of CO with combined femtosecond single- and dual-color laser pulses has been theoretically studied. The effect of the delay time between the femtosecond single- and dual-color laser pulses is discussed, and the physical mechanism of the enhancement of molecular orientation with pre-alignment of the molecule is investigated. It is found that the basic mechanism is based on the creation of a rotational wave packet by the femtosecond single-color laser pulse. Furthermore, we investigate the interference between multiple rotational excitation pathways following pre-alignment with femtosecond single-color laser pulse. It is shown that such interference can lead to an enhancement of the orientation of CO molecule by a factor of 1.6.

Keywords: molecular orientation, femtosecond dual-color laser pulse, quantum interference

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1. Introduction

Controlling rotation degrees of freedom of gas-phase molecules has been an important subject in the study of reaction dynamics and photochemistry as it provides a way to overcome the averaging over randomly oriented molecules. It is classified into two types: alignment and orientation. Perfect alignment implies that a molecular axis is completely parallel to a space fixed axis. Perfect orientation implies not only perfect alignment, but also that the molecular dipole moment points in the same direction as a chosen oriented spaced fixed axis.[1–4] Molecular alignment has become popular in revealing molecular structures,[5–7] controlling and tracing chemical reactions,[8–10] generating high-order harmonics from aligned molecules,[11–13] compressing optical pulses,[14] modulating THz generation,[15,16] generating few-cycle pulse generation,[17] and measuring ultrashort laser pulses based on the M-XFROG.[18–20]

Compared to the tremendous progress in molecular alignment mentioned above, the molecular orientation with distinguishable "head versus tail" orders is much more challenging but needed for various applications such as chemical reaction control[21] and molecular nanomaterial design.[22] In order to realize molecular orientation, several methods based on inducing an asymmetric potential with respect to the angle between the molecular axis and the laser polarization and breaking angular symmetry so as to achieve molecular orientation have been theoretically[23–33] and experimentally[34–40] studied. The basis mechanism is based on the creation of a rotational wave packet which consists of a superposition of rotational states with even and odd angular momentum quantum numbers J.[41]

Recently, it was experimentally shown that molecular orientation can be realized using femtosecond (fs) two-color laser pulse.[35,36] Furthermore, the enhancement of field-free molecular alignment and orientation could be obtained though pre-alignment of the molecule.[42–46] In this paper, we theoretically investigate the field-free molecular orientation with combined fs single- and dual-color laser pulses, with the CO molecule as an example. We first discuss the effect of the delay time between the fs single- and dual-color on molecular orientation. Then, we track the populations of the rotational states to demonstrate the physical mechanism of the enhancement of molecular orientation due to the pre-alignment of the molecule and find that the basic mechanism is based on the creation of a rotational wave packet by fs single-color laser pulse. Finally, we analyze the role of quantum interference between multiple excitation pathways.

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2. Theoretical method

We consider the control of a linear molecule by use of a hybrid laser pulse with the combination of single- and dual-color laser pulses given by

$$\begin{aligned} E(t) &= E_{\rm s}\exp\left(-2\ln 2\frac{t^2}{\tau_{\rm s}^2}\right)\cos\omega_{\rm s}t \\ &\quad + E_{\rm d}\exp\left(-2\ln 2\frac{(t-\Delta t)^2}{\tau_{\rm d}^2}\right) \\ &\quad \times\left[\cos\omega_{\rm d}t+\cos\left(2\omega_{\rm d}t+\phi\right)\right], \end{aligned} \tag{1}$$

where $\omega_{\rm s}$ and $\omega_{\rm d}$ are the carrier wave frequency, $E_{\rm s}$ and $E_{\rm d}$ are the field amplitude, $\tau_{\rm s}$ and $\tau_{\rm d}$ are the pulse duration, Δt is the delay time between the fs single- and the dual-color laser pulse. ϕ is the phase of the fs dual-color laser pulse, which determines the electric field structure of the fs dual-color laser pulse. When a linear molecule is exposed to the hybrid laser field $E(t)$, the time-dependent Schrödinger equation can be expressed based on a rigid-rotor model as[26]

$$\begin{aligned} {\rm i}\hbar\frac{\partial\Psi(\theta,t)}{\partial t} &= \Big[H_0+V_\mu(\theta)E(t)+V_{\rm pol}(\theta)E^2(t) \\ &\quad +V_{\rm hyp}(\theta)E^3(t)\Big]\Psi(\theta,t), \end{aligned} \tag{2}$$

with

$$H_0 = B\hat{J}^2, \tag{3}$$

$$V_\mu(\theta) = -\mu\cos\theta, \tag{4}$$

$$V_{\rm pol}(\theta) = -\frac{\left(\alpha_\parallel-\alpha_\perp\right)\cos^2\theta+\alpha_\perp}{2}, \tag{5}$$

$$V_{\rm hyp}(\theta) = -\frac{\left(\beta_\parallel-3\beta_\perp\right)\cos^3\theta+3\beta_\perp\cos\theta}{6}, \tag{6}$$

where B is the rotational constant, J^2 denotes the squared angular momentum operator, μ is the permanent dipole moment, θ is the angle between the molecular axis and the laser polarization, $\alpha_\parallel$ and $\alpha_\perp$ are the polarizability components parallel and perpendicular to the molecular axis, and $\beta_\parallel$ and $\beta_\perp$ are the hyperpolarizability components parallel and perpendicular to the molecular axis. The centre frequencies of the single- and dual-color laser pulse $\omega_{\rm s}$ and $\omega_{\rm d}$ are both set to be 12500 cm^{-1}, corresponding to the laser centre wavelength of 800 nm.

We expand the rotational wave function using the finite basis set of $|J,M\rangle$, which is a set of the eigenfunctions of a rigid rotor in a field-free space. Because we defined the polarization axes of the laser pulse as the laboratory-fixed Z axis, the Hamiltonian is cylindrically symmetric about the Z axis. Therefore, the magnetic quantum number M is conserved, that is $\Delta M = 0$, and then the wave function is expressed as

$$|\psi(t)\rangle = \sum_{J=0}^{J_{\max}} c_{J,M}(t)\,|J,M\rangle\exp\left(-{\rm i}\frac{E_J}{\hbar}t\right), \tag{7}$$

where $J_{\max}$ is set at the value which far exceeds the highest rotational states excited by the fs laser pulse, and E_J is an eigenenergy of the $|J,M\rangle$ state, which depends on J and not on M. By inserting the Hamiltonians in Eqs. (3)–(6) and the wave function in Eq. (7) into Eq. (1), it can be recast as an ensemble of coupled differential equations about the coefficient $c_{J,M}$. We solve these equations by applying the split-operator method.[47,48]

The molecular alignment and orientation dynamics can be estimated from the obtained wave function as follows:

$$\begin{aligned} \langle\cos\theta\rangle(t) &= \sum_{J=0}^{J_{\max}}\sum_{J'=0}^{J'_{\max}}\left|c_{J',M}c_{J,M}\right|\langle J',M|\cos\theta\,|J,M\rangle \\ &\quad\times\exp\left[{\rm i}\left(\frac{\Delta E_{J',J}}{\hbar}t-\varphi_{J',J}\right)\right] \\ &= 2\sum_{J=0}^{J_{\max}}\left|c_{J+1,M}c_{J,M}\right|\langle J+1,M|\cos\theta\,|J,M\rangle \\ &\quad\times\cos\left(\frac{\Delta E_{J+1,J}}{\hbar}t-\varphi_{J+1,J}\right), \end{aligned} \tag{8}$$

where we use the evaluations of matrix elements $\langle J',M|\cos\theta\,|J,M\rangle$ when $|J'-J|\neq 1$, employing properties of spherical harmonics the following notations:

$$\Delta E_{J+1,J} = E_{J+1}-E_J = 2B(J+1), \tag{9}$$

$$\varphi_{J+1,J} = \arg(c_{J+1,M})-\arg(c_{J,M}). \tag{10}$$

From Eq. (8), it is obvious that the orientation dynamics includes several frequency components that correspond to energy differences between neighboring rotational states and the orientation dynamics is determined by the modulation amplitude of each component $|c_{J+1,M}c_{J,M}|$ and the relative phase between rotational states $\varphi_{J+1,J}$.

3. Numerical results and discussion

Based on the method described in the previous section, we performed simulations using CO as the target molecule. The molecular parameters of the CO molecule are μ = 0.112 D, $\alpha_\parallel = 2.294$ Å^3, $\alpha_\perp = 1.77$ Å^3, $\beta_\parallel = 2.748\times10^9$ Å^5, and $\beta_\perp = 4.994\times10^8$ Å^5.[49,50] The rotational constant in its vibronic ground state and the rotational period are B = 1.93 cm^{-1} and $T_{\rm rot}\approx 8.642$ ps. In the calculations, we use a fs single-color laser pulse with a peak intensity of 5.0×10^{13} W/cm^2 and pulse duration of 100 fs in intensity. The intensity and pulse duration of the dual-color laser pulse is the same as that of the single-color laser pulse and the phase $\phi = 0$.

Figure 1 shows the calculated results of molecular orientation obtained by assuming that the CO molecule is initially in its ground rotational state $|J=0,M=0\rangle$. The horizontal axis in Fig. 1(a) represents the time delay of the single-color laser pulse with respect to the dual-color laser pulse. The vertical axis represents a moment at which we define the envelop

peak of the dual-color as an origin of the coordinate. The two dashed lines in Fig. 1(b) illustrate the maximum degrees of the positive and negative orientation created by only the dual-color laser pulse. The molecular orientation created by the single- and dual-color laser pulses is studied in a time delay over a full rotational period, and thus all kinds of cases can be included. The maximum degree of negative value under field-free conditions reaches $\langle\cos\theta\rangle_{\min} = -0.785$ at the delay time of $\Delta t = 4.24$ ps denoted by A in Fig. 1(b) and the time of 13.66 ps. In our simulations, $\langle\cos\theta\rangle < 0$ corresponds to the case when the C atoms are directed in the positive direction of the laboratory-fixed Z axis, i.e., the positive direction of the fs two-color laser fields. The maximum degree of positive value, which corresponds to the C atom directed in negative direction, is determined to be $\langle\cos\theta\rangle_{\max} = 0.727$. Thus, the orientation dynamics is asymmetric. The only way to achieve $\langle\cos\theta\rangle_{\max} = 0.785$ is to reverse the sign of the dual-color field (that is $\phi = \pi$). We performed another simulation with the same parameters but without the single-color laser pulse. In this case, the maximum orientation parameter is $|\langle\cos\theta\rangle|_{\max} = 0.540$. Thus, we conclude that the pre-excitation with the single-color laser pulse enhances the degree of molecular orientation.

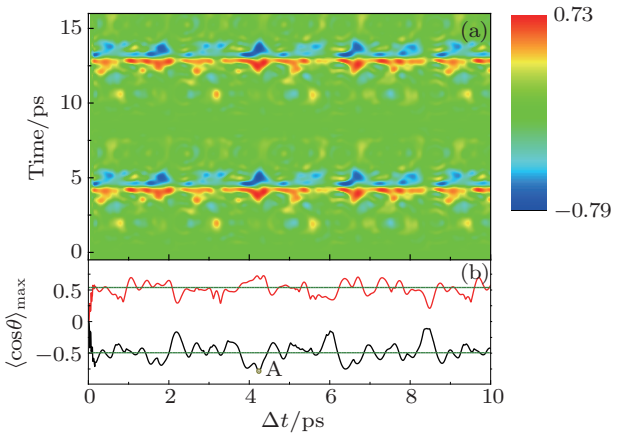


Fig. 1. (color online) (a) Two-dimensional plot of orientation dynamics with respect to the time delay Δt between the fs single- and dual-color laser pulses (x axis), and the time after the peak intensity of the fs dual-color laser pulse (y axis) in the upper panel. (b) The maximum degree of positive and negative molecular orientation with respect to the the time delay Δt. The optimal time delay $\Delta t = 4.24$ ps, denoted by A.

Figure 2 shows the calculated results when the delay time between the single- and dual-color pulses is $\Delta t = 4.24$ ps (denoted by A in Fig. 1(b)) and the parameters of the single- and dual-color laser pulse are the same as that in Fig. 1. Figure 2(a) shows the time-dependent angular distribution. Figures 2(b) and 2(c) display the time evolution of the molecular alignment $\langle\cos^2\theta\rangle$ and molecular orientation $\langle\cos\theta\rangle$. We can see that the molecular alignment and orientation reaches its peak shortly after the dual-color laser pulse and recurs at full rotational periods $t = nT_{\rm rot}$, where n is an integer number, and $T_{\rm rot}$ is the rotational period of the CO molecule with $T_{\rm rot} \approx 8.642$ ps, as shown in Figs. 2(b) and 2(c). It can be seen from Figs. 2(b) and 2(c) that the maximum degrees of alignment and the negative orientation value under field-free conditions reach 0.887 and −0.785, respectively. The molecular alignment and orientation value do not reach the maximum at the same time.

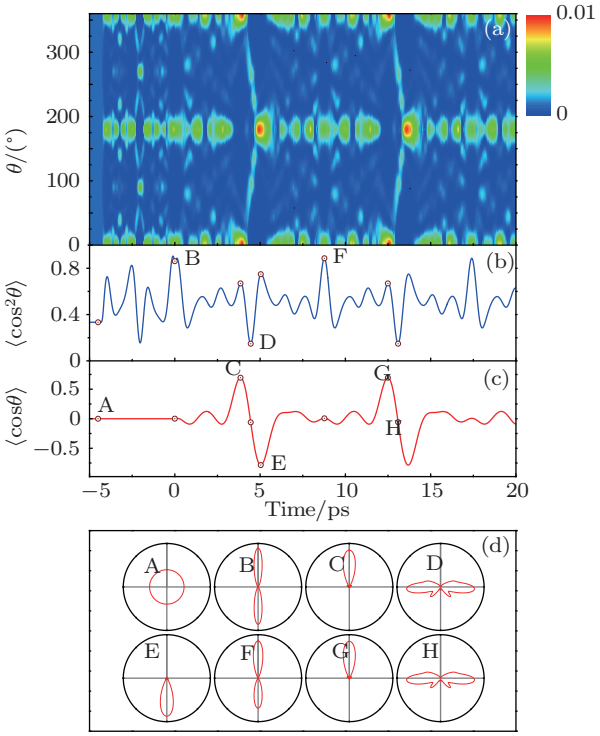


Fig. 2. (color online) (a) Time-dependent angular distribution, (b) time evolution of molecular alignment $\langle\cos^2\theta\rangle$, (c) time evolution of molecular orientation $\langle\cos\theta\rangle$, and (d) polar plot representation of the angular distribution at different times indicated in (b) and (c) for an ensemble of CO molecules by the combined fs single- and dual-color laser pulses when time delay $\Delta t = 4.24$ ps. The linear polarizations of the fs two-color laser pulse are aligned vertically in the plane of the figure.

In order to give an intuitive explanation of field-free molecular alignment and orientation, polar plot representation of angular distributions of the rotational wave packets at the times denoted by A–H in Figs. 2(b) and 2(c) is depicted in Fig. 2(d). The angular distributions display a rich variety of spatial asymmetries with periodic inversion which indicates that the rotational wave packet evolves freely after the kicks are over and the evolution of the field-free alignment and orientation depends on the distribution of rotational states. As shown in Figs. 2(b) and 2(c), the fs dual-color laser pulse is applied when the molecular alignment almost reach its maximum (marked as B), which is opposite to the case of half-cycle[44] and THz[46] laser pulses. At C and E, the maximum degree of molecular orientation reaches a negative value with $\langle\cos\theta\rangle_{\max} = 0.694$ and positive with $\langle\cos\theta\rangle_{\min} = -0.785$. Interestingly, the transition between $\langle\cos\theta\rangle_{\max}$ and $\langle\cos\theta\rangle_{\min}$ is very fast compared to the time scale of rotational dynamics. At D, the molecules are anti-aligned and $\langle\cos\theta\rangle = 0.148$. In addition, it should be noted that the achieved orientation in

Fig. 2(c) has a finite duration of 660 fs for $|\langle\cos\theta\rangle|_{\max} > 0.5$. From the viewpoint of applications, the achieved duration is long enough to probe electron dynamics via photoemission or high-order harmonic generation, or vibrational dynamics using fs laser pulses.

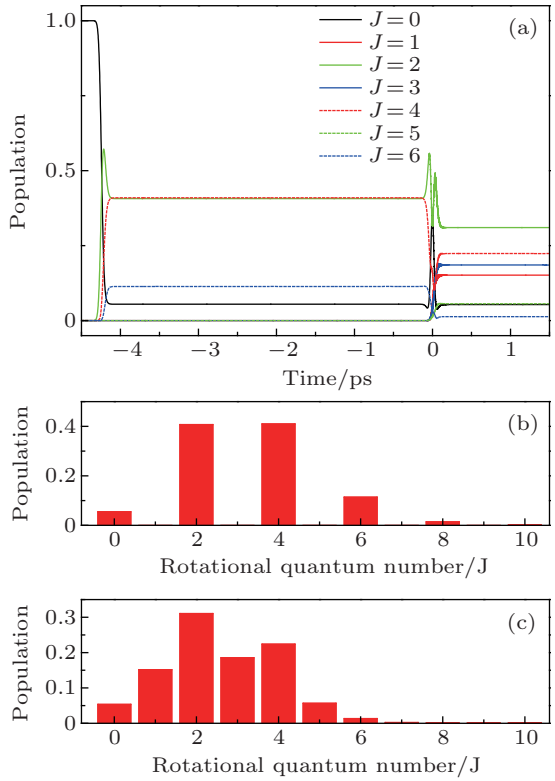


Fig. 3. (color online) (a) Time-evolution of the populations of rotational states under the action of the combined fs single- and dual-color laser pulse. (b) The rotational state distribution after the interaction with the fs single-color laser pulse and before the fs dual-color laser pulse. (c) The rotational state distribution after the interaction with the fs dual-color laser pulse. The parameter of the fs single- and dual-color laser pulses are the same as that of Fig. 2.

To demonstrate the physical mechanism of the enhancement of molecular orientation with pre-alignment of molecule, we further track the populations of the rotational states. Figure 3(a) shows the time evolution of the populations of rotational states when the delay time $\Delta t = 4.24$ ps. First, the molecules are excited to $J = 2$, 4, 6, 8 states by the fs single-color laser pulse and then transferred to $J = 1$, 3, 5, 7 by the fs dual-color laser pulse as shown in Figs. 3(b) and 3(c). After the irradiation of both pulses, the populations remain unchanged and the ratio of each rotational state is shown in Fig. 3(c). As shown in Fig. 2(c), there is no molecular orientation before the dual-color laser pulse. Therefore, the fact that the dual-color laser pulse including a DC component can induce molecular orientation is because that it can change the parity of the molecular rotational wave function and both even and odd rotational states are excited. The molecular alignment and orientation degree, depending on both populations and relative phases, change with time, as plotted in Figs. 2(b) and 2(c). This is a signature of coherent excitation and quantum interference. The aligned molecule consists of a coherent superposition of rotational states ($J = 0$, 2, 4, 6, ..., see Fig. 3(b)) with time-dependent phase factors. The final orientation depends on the interference between these states induced by the dual-color laser pulse. In order to show the importance of quantum interference between pairs of pathways, we calculate an incoherent average of the orientation over the rotational distribution in Fig. 3(b), as shown in Fig. 4. Comparing with the result in Fig. 2(c), we deduce that the orientation can be enhanced by a factor close to 1.6 due to quantum interference.

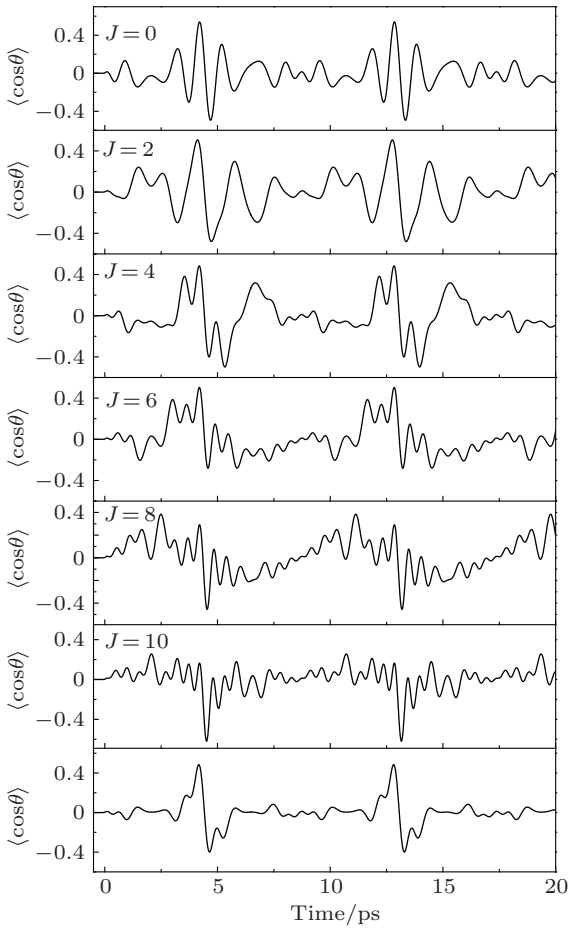


Fig. 4. The degree of field-free orientation $\langle\cos\theta\rangle$ for different initial rotation quantum number: (a) $J = 0$, (b) $J = 2$, (c) $J = 4$, (d) $J = 6$, (e) $J = 8$, and (f) $J = 10$. Panel (g) shows the overall orientation after the fs dual-color laser pulse as an incoherent averaged over the rotational distribution in Fig. 3(b).

4. Conclusion

We theoretically study the coherent control of field-free molecular orientation of CO with combined fs single- and dual-color laser pulses and find that the fs dual-color laser pulse can orient molecules because it can change the parity of molecular rotation wave function, and thus both the even and the odd rotational states are excited. We discuss the effect of the delay time between fs single- and dual-color on

molecular orientation and find that the optimal delay time is $\Delta t = 4.24$ ps. Then we track the populations of the rotational states to demonstrate the physical mechanism of the enhancement of molecular orientation with pre-alignment of molecule and find that the basic mechanism is based on the creation of a rotational wave packet by fs single-color laser pulse which consists of a superposition of rotational states. Finally, the role of quantum interference between multiple excitation pathways is quantified.

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