ISSN 1674-1056
http://cpb.iphy.ac.cn
http://iopscience.iop.org/cpb
中国物理 B
Chinese Physics
中国物理 Chinese Physics B

Quantum interference of multi-orbital effects in high-harmonic spectra from aligned carbon dioxide and nitrous oxide

Hong-Jing Liang(梁红静), Xin Fan(范鑫), Shuang Feng(冯爽), Li-Yu Shan(单立宇), Qing-Hua Gao(高庆华), Bo Yan(闫博), Ri Ma(马日), Hai-Feng Xu(徐海峰)
Citation: Chin. Phys. B . 2019, 28(9): 094207 . **doi:** 10.1088/1674-1056/28/9/094207
Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

What follows is a list of articles you may be interested in

Resolving multi-orbital effects on high harmonic generation from aligned N_2 molecules in linearly and elliptically polarized intense laser fields

Hong-Jing Liang(梁红静), Xin Fan(范鑫), Shuang Feng(冯爽), Li-Yu Shan(单立宇), Qing-Hua Gao(高庆华), Bo Yan(闫博), Ri Ma(马日), Hai-Feng Xu(徐海峰), Da-Jun Ding(丁大军)
Chin. Phys. B . 2019, 28(9): 094211 . **doi:** 10.1088/1674-1056/28/9/094211

Femtosecond enhancement cavity with kilowatt average power

Jin Zhang(张津), Lin-Qiang Hua(华林强), Shao-Gang Yu(余少刚), Zhong Chen(陈忠), Xiao-Jun Liu(柳晓军)
Chin. Phys. B . 2019, 28(4): 044206 . **doi:** 10.1088/1674-1056/28/4/044206

Effect of multiple rescattering processes on harmonic emission in spatially inhomogeneous field

Cai-Ping Zhang(张彩萍), Chang-Long Xia(夏昌龙), Xiang-Fu Jia(贾祥富), Xiang-Yang Miao(苗向阳)
Chin. Phys. B . 2018, 27(3): 034206 . **doi:** 10.1088/1674-1056/27/3/034206

Spectral redshift of high-order harmonics by adding a weak pulse in the falling part of the trapezoidal laser pulse

Xue-Fei Pan(潘雪飞), Jun Zhang(张军), Shuai Ben(贲帅), Tong-Tong Xu(徐彤彤), Xue-Shen Liu(刘学深)
Chin. Phys. B . 2018, 27(2): 024206 . **doi:** 10.1088/1674-1056/27/2/024206

Laser phase effect on asymmetric harmonic distribution in H_2^+

Li-Qiang Feng(冯立强), Wen-Liang Li(李文亮), Hui Liu(刘辉)
Chin. Phys. B . 2017, 26(4): 044206 . **doi:** 10.1088/1674-1056/26/4/044206

SPECIAL TOPIC — Strong-field atomic and molecular physics

Quantum interference of multi-orbital effects in high-harmonic spectra from aligned carbon dioxide and nitrous oxide*

Hong-Jing Liang(梁红静), Xin Fan(范鑫), Shuang Feng(冯爽), Li-Yu Shan(单立宇), Qing-Hua Gao(高庆华), Bo Yan(闫博), Ri Ma(马日)†, and Hai-Feng Xu(徐海峰)‡

Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, *China*

(Received 27 May 2019; revised manuscript received 24 June 2019; published online 20 August 2019)

We investigate experimentally multi-orbital effects in high-order harmonic generation (HHG) from aligned CO_2 and N_2O molecules by intense femtosecond laser fields with linear and elliptical polarizations. For either of the aligned molecules, a minimum in the harmonic spectrum is observed, the position of which shifts to lower-order harmonics when decreasing the intensity or increasing the ellipticity of the driving laser. This indicates that the minimum originates from the dynamic interference of different channels, of which the tunneling ionization and recombination are contributed via different molecular orbitals. The results show that both the highest occupied molecular orbital (HOMO) and low-lying HOMO-2 in CO_2 (or HOMO-1 in N_2O) contribute to the molecular HHG in both linearly and elliptically polarized strong laser fields. Our study would pave a way for understanding multi-electron dynamics from polyatomic molecules irradiated by strong laser fields.

Keywords: high-order harmonic generation, aligned molecule, multi-orbital effect, dynamic interference

PACS: 42.65.Ky, 33.80.–b, 33.80.Rv **DOI:** 10.1088/1674-1056/ab3438

1. Introduction

The interaction of strong laser radiation with atoms or molecules results in various non-perturbative and highly nonlinear phenomena, such as high-order above threshold ionization (HATI),[1,2] non-sequential double (NSDI) and multiple ionization,[3] neutral high Rydberg state excitation (RSE),[4] and high-order harmonic generation (HHG).[5,6] Among them, HHG has attracted intense research interest, due to its potential applications as tabletop coherent radiation source in the extreme ultraviolet (XUV) and soft x-ray regions,[7] as well as attosecond pulses.[8–12] HHG facilitates measurements that could resolve electronic structure[13,14] and dynamic processes[15,16] on sub-femtosecond time scale and with sub-nanometer spatial resolution.

The physical picture of atomic HHG in a strong laser field is a well-known semi-classical three-step model:[17] (i) tunneling ionization of electrons in an atom or molecule, (ii) the quasi-free electrons are accelerated in the intense laser field, (iii) the high energy electrons recombine with the ionic core to emit redundant energy as coherent XUV photon flux. Molecules have much more complicated structures than atoms, which have multicenter and diverse geometric structure, large density of electronic states with different symmetries, as well as additional nuclear rotational and vibrational motions, providing extra parameters to control HHG.[18–20] By studying HHG of aligned molecules, several experimental and theoretical observations[21–25] have identified that both ionization and recombination are dependent on the symmetries of the highest occupied molecular orbital (HOMO) and even lower-lying molecular orbitals (HOMO-1, HOMO-2, ...). Based on the underlying physics of HHG from molecules, there are some approaches on ultrafast imaging of molecular orbitals. Itatani *et al.*[13] in their experiments reported for the first time the tomographic reconstruction of HOMO from aligned N_2 molecules. Baker *et al.*[26] used molecular HHG to detect the ultrafast motions of protons of H_2 and CH_4 with attosecond temporal resolution. The internuclear distance of molecule can also be analyzed by observing the two-center interference minimum of HHG spectra.[14,27] Nevertheless, some other mechanisms of HHG from polyatomic molecules are still kept ambiguous, such as Coulomb field influence and multiple orbital coupling.

Here we experimentally investigate and compare the HHG spectra from aligned triatomic molecules CO_2 and N_2O by femtosecond strong laser field. While both molecules are linearly structured, N_2O is asymmetry triatomic molecules with a $C_{\infty v}$ symmetry which has a permanent dipole moment. On the other hand, both molecules have same numbers of electrons and nearly identical internuclear distance ($R_{C–O} = 1.16$ Å in CO_2, $R_{N–N} = 1.186$ Å, $R_{N–O} = 1.126$ Å in N_2O), as well as similar HOMO orbitals. A comparison study

*Project supported by the National Natural Science Foundation of China (Grant Nos. 91750104, 11534004, 11874179, 11127403, 11474130) and the Natural Science Foundation of Jilin Province, China (Grant No. 20180101289JC).

†Corresponding author. E-mail: rma@jlu.edu.cn

‡Corresponding author. E-mail: xuhf@jlu.edu.cn

© 2019 Chinese Physical Society and IOP Publishing Ltd

on harmonic spectra of aligned N_2O and CO_2 would add more knowledge to the molecular structure effect on HHG in strong laser fields.

There are some studies that have been reported on the molecular structure and multi-electron dynamics of HHG from CO_2 or N_2O.[15,28–30] Smirnova *et al.*[15] have reported the minimum position of the HHG spectra in CO_2 molecules which is related to the intensity of the driving laser. This observation is interpreted in terms of the destructive interference from different molecular orbitals (HOMO and HOMO-2) for high-harmonic emission. Wörner *et al.*[28] have observed that the positions of the minima of harmonic spectra from aligned CO_2 shifted by over more than 15 eV with the change of both wavelength and intensity of the driving laser. Rupenyan *et al.*[29] investigated the effects of electronic structures and multi-electron dynamics on the harmonic spectra from CO_2 and N_2O by using near-infrared driving laser fields in the wavelength range of 1.17–1.46 μm. The results indicated that the minimum of harmonic spectrum driven by laser fields with shorter wavelength (1.17 μm) would be located at higher-order harmonics near the cut-off region, while changing to the driving laser field with a longer wavelength (1.36 and 1.46 μm), the minimum of harmonic spectrum would be distinctly positioned in the plateau region. Recently, Monfared *et al.*[30] performed a theoretical study on the effects of inner orbitals and multiple electrons on the harmonic spectrum. These elaborated studies indicated that both the molecular orbital structure and the interference of multi-orbitals affect the minimum position of HHG. The fact that the position of the minimum is controllable by the intensity and wavelength of the driving laser is now understood by the destructive interference between different channels in ionization and recombination processes of HHG. The majority of previous studies are performed by using the driving laser with linear polarization. Comparing to linearly polarized laser field, the freed electron dynamics during HHG process can be tuned by controlling the laser field ellipticity. The elliptically polarized driving laser field would provide additional freedom degrees to control the high harmonic generation. For example, Mairesse *et al.*[31] experimentally and theoretically investigated the HHG of aligned CO_2 and N_2 molecules in elliptically polarized laser field, the results of which show that the electron wavepacket can be controlled in the process of HHG.

In our study, we investigate and compare HHG of aligned CO_2 and N_2O molecules in both linearly and elliptically polarized laser field. The harmonic yield is measured with different intensity and ellipticity of the driving laser field. Based on our experimental observations, we discuss the multi-orbital effects and multi-electronic dynamics on HHG from aligned CO_2 and N_2O in strong laser fields.

2. Experiments

The experimental setup used for generation and detection of HHG has already been described in our previous work.[32–34] Briefly, a Ti: sapphire laser system operating at 1 kHz repetition was used to deliver ∼ 35 fs pulses centered at 800 nm. The output pulse is divided into two parts by using a 30 : 70 beam splitter. One laser beam with lower energy (aligning laser) was used to excite rotational energy levels and form rotational wave packets of CO_2 or N_2O molecules. The other beam with higher energy (driving laser) was used to drive the aligned molecules to generate harmonics. The ellipticity of the driving laser was changed by a combination of an adjustable zero-order half-wave plate placed before a zero-order quarter-wave plate with fixed optic axis. This configuration minimizes the diffraction efficiency of spherical grating affected by the polarization of HHG. A motorized delay stage was inserted into the path of driving laser to control the relative delay time between the two laser pulses. A half-wave plate and a Glan-laser polarizer were placed in the path of each laser beam to adjust its intensity. The polarization angle Θ between the aligning and driving lasers was adjusted by using a half-wave plate placed in the path of the aligning laser. After focused by a focal length 300 mm, the aligning laser and the driving laser were collinearly sent into the gas zone to align the molecules and generate harmonics. The intensity of the aligning laser at the interaction region was about 7×10^{13} W/cm^2. The backing pressure of CO_2 or N_2O (gas purity at 99.999%) gases was 2 bar. The gaseous samples were continuously expanded into the interaction vacuum chamber through a 100 μm orifice, leading to the density of gas was about 10^{17} cm^{-3} and the rotational temperature was estimated to be ∼ 100 K. The harmonics generated in the gas zone were spectrally dispersed by a spherical grating with a groove density of 1200 groves/mm and then focused onto a microchannel plate detector attached with a phosphor screen. A CCD camera was used to image the phosphor screen and transferred to a computer.

3. Results and discussion

In our study, we investigate the harmonics from aligned molecules by varying the driving laser intensity and polarization, which would add our understanding on the multi-orbital effect of molecular HHG. We first investigate the alignment of molecules by measuring the harmonic intensities on the delay time between the aligning and driving lasers. The polarization of the two lasers are set to be parallel to each other. The results for the 27th harmonics for CO_2 and N_2O molecules are shown in Fig. 1(a) and Fig. 1(b), respectively. The duration of the aligning pulse (35 fs) used in the experiments is much shorter than the rotational period of each molecule (T_{rot} = 42.7 ps of CO_2 and T_{rot} = 39.8 ps of N_2O). The ultrashort aligning

pulse will excite the randomly oriented molecules to form rotational wave packets.[35,36] As the rotational wave packets evolve in time, the molecules will be aligned periodically with the molecular axis parallel or perpendicular to the polarization of the aligning laser. The effect of such non-adiabatic impulsive alignment on molecules is reflected in the modulation of harmonic intensity, as shown in Fig. 1. To reduce the effect of instrumental response for qualitative comparison, we use the ratio S/S_0 to represent the harmonic intensity throughout the study, i.e., the measured harmonic intensity (S) from aligned molecules normalized to that from nonaligned molecules (S_0). As shown in Fig. 1(a), obvious modulation of the harmonic intensity of CO_2 molecule occurs at a delay time of ~ 21 ps and ~ 42 ps, corresponding to $T_{\rm rot}/2$ (half rotational revival) and $T_{\rm rot}$ (full rotational revival), respectively. The half and full revivals are also evident for N_2O molecules (Fig. 1(b)), while the 1/4 and 3/4 periods of revival are much weaker due to nuclear spin statistics.[37] In the following experiments, the delay time of alignment is fixed at 21.1 ps and 19.7 ps for CO_2 and N_2O molecules, respectively. That is, the molecular axis is aligned parallel to the polarization of the aligning laser.

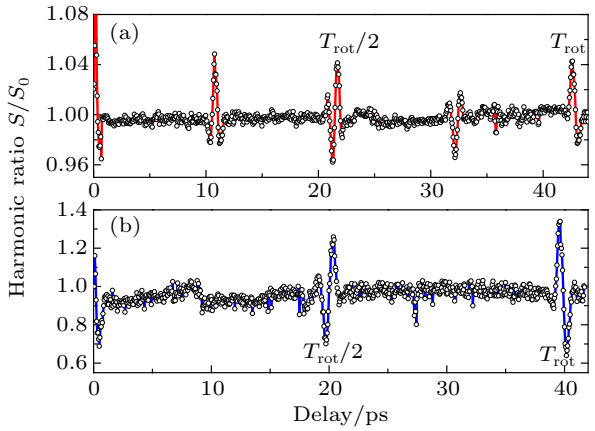


Fig. 1. Ratio of the 27th harmonic intensity between aligned (S) and unaligned (S_0) samples of CO_2 (a) and N_2O (b) molecules as a function of the delay time between the two laser beams. The polarization of the driving laser is parallel to that of the aligning laser. The $T_{\rm rot}/2$ (half revival) and $T_{\rm rot}$ (full revival) are indicated in the figure.

In Fig. 2, we show the measured harmonic intensity of each order by changing the driving laser intensity in the range of 1.2×10^{14} W/cm^2 to 2.0×10^{14} W/cm^2 for aligned CO_2 (Fig. 2(a)) and N_2O (Fig. 2(b)) molecules. For either of the molecules, a minimum in the harmonic spectrum is clearly observed, which shifts to higher-order harmonics when increasing the laser intensity. For CO_2, the minimum shifts from H23 at 1.2×10^{14} W/cm^2 to H29 at 2.0×10^{14} W/cm^2, and for N_2O, from H23 to H27. The results of CO_2 reproduce previous experimental studies by Smirnova *et al.*[15] and Wörner *et al.*,[28] while the experimental results of N_2O are similar to those of Rupenyan *et al.*[29] Such minimum in harmonic spectrum is interpreted by the destructive interference of different channels induced by tunneling ionization from different molecular orbitals.[15] The structures of HOMO and lower-lying orbitals (HOMO-1 and HOMO-2) of CO_2 and N_2O are presented in Fig. 3, which are calculated by the density functional theory (DFT) method at the B3LYP/6-311++G** level with Gaussian 03[38] program and are plotted with Multiwfn package.[39] The HOMO, HOMO-1, and HOMO-2 of CO_2 molecule exhibit π_g, π_u, and σ_u symmetry, respectively (Figs. 3(a)–3(c)). Since the CO_2 molecule is aligned parallel to the driving laser polarization, the tunneling ionization and recombination of HOMO-1 could be negligible, since the electron density distribution of the orbital has a nodal plane along the molecular axis (see Fig. 3(b)). It has been demonstrated that in this case, the destructive interference in HHG of CO_2 is induced by the contributions of both HOMO and HOMO-2.[15] For N_2O, the symmetry of HOMO is similar to that of CO_2, that of HOMO-1 is a σ orbital, which is like the structure of HOMO-2 of CO_2, and HOMO-2 exhibits a nodal plane along the molecular axis (Figs. 3(d)–3(f)). Thus, this indicates that when the molecule is aligned parallel to the laser polarization, the destructive interference between the channels of HOMO and HOMO-1 results in the observed minimum in harmonic spectrum of N_2O shown in Fig. 2(b).

The effect of such destructive interference, also known as dynamic interference, replies on the phase difference of HHG from the two different channels. The phase is determined by

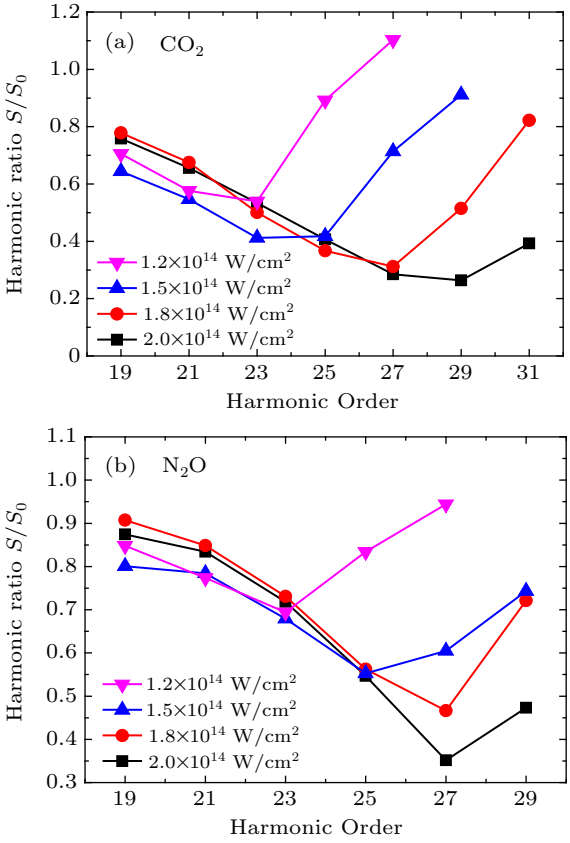


Fig. 2. HHG ratios measured with (s) and without (S_0) the aligning laser in CO_2 (a) and N_2O (b) as a function of harmonic order in linearly polarized driving laser with different intensities (1.2, 1.5, 1.8, and 2.0) $\times10^{14}$ W/cm^2, respectively.

the delay time between the tunneling ionization and recombination, which depends on the intensity of the driving laser field. Thus the minimum in harmonic spectrum shifts as the laser intensity is changed. The intensity-dependent interference from different channels in HHG of CO_2 molecules has been discussed in detail in the pioneer paper by Smirnova *et al.*[15] The results in Fig. 2(b) show that similar phenomenon exists in the HHG of aligned N_2O molecules. Our study further demonstrates that the minimum in HHG is common in molecules, which depend on the intensity of linearly polarized driving laser field and reflect the characteristic of dynamic interference from different molecular orbitals.

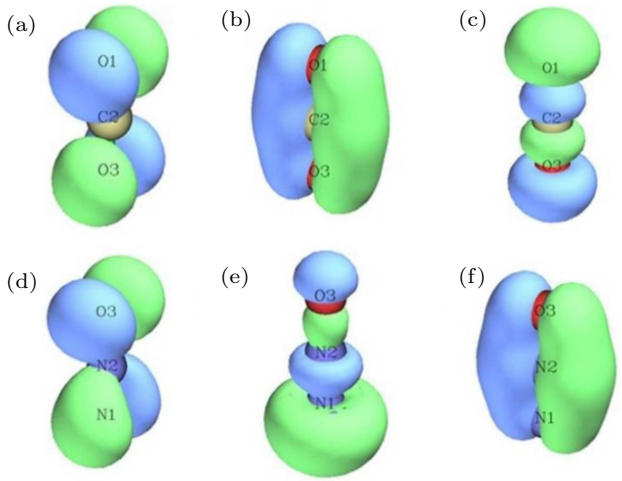


Fig. 3. Orbital structures of HOMO, HOMO-1, and HOMO-2 of CO_2 (a)–(c) and N_2O (d)–(f) calculated by the DFT method at the B3LYP/6-311++G** level.

We further investigate the harmonic intensities from aligned CO_2 and N_2O molecules in elliptically polarized driving laser field. Figure 4 presents the harmonic ratio S/S_0 with the ellipticity of the driving laser $\varepsilon = 0.18$ or $\varepsilon = 0.36$ for aligned CO_2 (Fig. 4(a)) and N_2O (Fig. 4(b)). The intensity of the driving laser is kept at 2.0×10^{14} W/cm^2 measured at the linear polarization ($\varepsilon = 0$). For either of the molecules, a noticeable shift of the minimum position toward lower-order harmonics can be seen for higher ellipticity of the driving laser. This finding can be understood in the following two concerns. Firstly, as we have mentioned above, the results of dynamic interference lead to the minimum appearing at lower order harmonics for lower driving laser intensity. The effective intensity (I) in an elliptically polarized laser will decrease comparing to that in a linearly polarized laser (I_0), $I = I_0/(1+\varepsilon^2)$. Thus one would expect the shift of the minimum in an elliptically polarized laser fields if the intensity I_0 is kept at a constant value. Secondly, the initial conditions of tunneling ionization would be different for that in a linearly polarized laser fields, since additional drift velocity would be induced in an elliptically polarized strong laser field.[40] This would also affect the recombination process to produce HHG, including the delay time between ionization and recombination. In their study, Larsen *et al.*[41] have shown that the electron excursion time τ of HHG, corresponding with the delay time between ionization and recombination, would be changed upon varying laser ellipticity ε. This fact would in turn affect the position of the dynamic interference minimum, since it is related to the excursion time τ.[15] As a consequence, the minimum in the harmonic spectrum would be changed because the dynamics interference between channels is dependent on the ionization and recombination processes. Our experimental results will stimulate further insight studies, both experimentally and theoretically, to reveal the detailed physics of the dynamic interference in an elliptically polarized strong laser field.

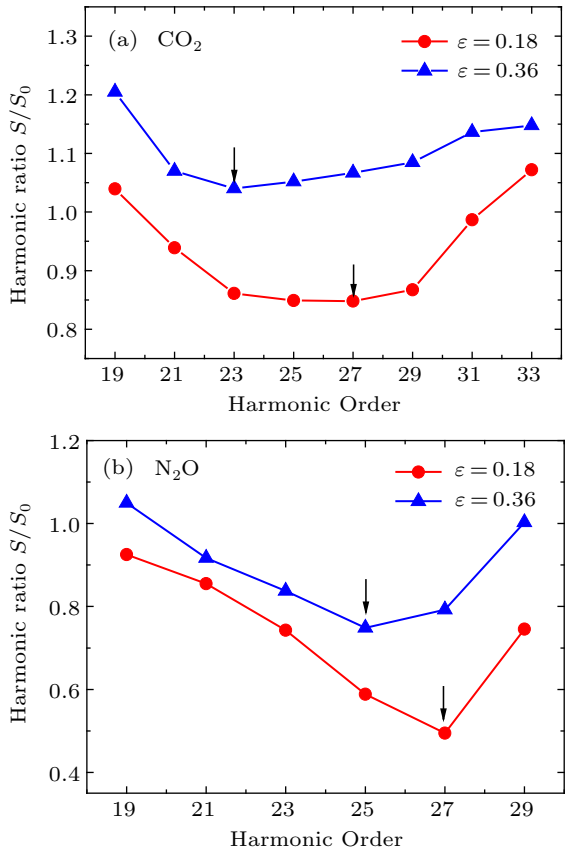


Fig. 4. Harmonic ratio S/S_0 of aligned CO_2 (a) and N_2O (b) with the ellipticities $\varepsilon = 0.18$ (red circles) and $\varepsilon = 0.36$ (blue triangles), respectively.

4. Conclusions

In this work, we have performed an experimental investigation on the multiple orbitals effect in the HHG from aligned CO_2 and N_2O molecules by both linearly and elliptically polarized strong laser field. The position of the minimum in the HHG spectra could be shifted by the intensity and ellipticity of driving laser. The reason was interpreted as the dynamic interference of HHG from the HOMO and HOMO-2 in CO_2 (or HOMO-1 in N_2O). Our research results would shed some light for further studies on the multi-orbital effect in the interaction of molecules with strong laser fields.

References

[1] Milošević D B, Paulus G G, Bauer D and Becker W 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** R203

[2] Zhang K, Liu M, Wang B B, Guo Y C, Yan Z C, Chen J and Liu X J 2017 *Chin. Phys. Lett.* **34** 113201

[3] Becker W, Liu X J, Ho P J and Eberly J H 2012 *Rev. Mod. Phys.* **84** 1011

[4] Nubbemeyer T, Gorling K, Saenz A, Eichmann U and Sandner W 2008 *Phys. Rev. Lett.* **101** 233001

[5] Macklin J J and Kmetec J D 1993 *Phys. Rev. Lett.* **70** 766

[6] Li X Z, Zhuo H B, Zou D B, Zhang S J, Zhou H Y, Zhao N, Lang Y and Yu D Y 2017 *Chin. Phys. Lett.* **34** 094201

[7] Sansone G, Benedetti E, Calegari F, Vozzi C, Avaldi L, Flammini R, Poletto L, Villoresi P, Altucci C, Velotta R, Stagira S, De S and Nisoli M 2006 *Science* **314** 443

[8] Zhao K, Zhang Q, Chini M, Wu Y, Wang X and Chang Z 2012 *Opt. Lett.* **37** 3891

[9] Li X Y, Wang G L and Zhou X X 2014 *Chin. Phys. B* **23** 013102

[10] Wu J S, Jia Z M and Zeng Z N 2017 *Chin. Phys. B* **26** 093201

[11] Li W, Wang G L and Zhou X X 2011 *Acta Phys. Sin.* **60** 123201 (in Chinese)

[12] Salehi M and Mirzanejad S 2017 *Chin. Phys. Lett.* **34** 054202

[13] Itatani J, Levesque J, Zeidler D, Niikura H, Pépin H, Kieffer J C, Corkum P B and Villeneuve D M 2004 *Nature* **432** 867

[14] Kanai T, Minemoto S and Sakai H 2005 *Nature* **435** 470

[15] Smirnova O, Mairesse Y, Patchkovskii S, Dudovich N, Villeneuve D, Corkum P and Ivanov M Y 2009 *Nature* **460** 972

[16] Li W, Zhou X, Lock R, Patchkovskii S, Stolow A, Kapteyn H C and Murnane M M 2008 *Science* **322** 1207

[17] Corkum P B 1993 *Phys. Rev. Lett.* **71** 1994

[18] Walters Z B, Tonzani S and Greene C H 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** F277

[19] Itatani J, Zeidler D, Levesque J, Spanner M, Villeneuve D M and Corkum P B 2005 *Phys. Rev. Lett.* **94** 123902

[20] Su N, Yu S J, li W Y, Yang S P and Chen Y J 2018 *Chin. Phys. B* **27** 054213

[21] Zhang J, Wu Y, Zeng Z and Xu Z 2013 *Phys. Rev. A* **88** 033826

[22] Zhou X X, Tong X M, Zhao Z X and Lin C D 2005 *Phys. Rev. A* **71** 061801

[23] Mcfarl B K, Farrell J P, Bucksbaum P H and Guhr M 2008 *Science* **322** 1232

[24] Li G H, Xie H Q, Yao J P, Chu W, Cheng Y, Liu X J, Chen J and Xie X H 2016 *Acta Phys. Sin.* **65** 224208 (in Chinese)

[25] Lin C D, Jin C, Le A T and Lucchese R R 2012 *J. Phys. B: At. Mol. Opt. Phys.* **45** 194010

[26] Baker S, Robinson J S, Haworth C A, Teng H, Smith R A, Chirilă C C, Lein M, Tisch J W G and Marangos J P 2006 *Science* **312** 424

[27] Vozzi C, Calegari F, Benedetti E, Caumes J P, Sansone G, Stagira S, Nisoli M, Torres R, Heesel E, Kajumba N, Marangos J P, Altucci C and Velotta R 2005 *Phys. Rev. Lett.* **95** 153902

[28] Wörner H J, Bertr J B, Hockett P, Corkum P B and Villeneuve D M 2010 *Phys. Rev. Lett.* **104** 233904

[29] Rupenyan A, Kraus P M, Schneider J and Wörner H J 2013 *Phys. Rev. A* **87** 033409

[30] Monfared M, Irani E and Sadighi-Bonabi R 2018 *J. Chem. Phys.* **148** 234303

[31] Mairesse Y, Dudovich N and Levesque J 2008 *New J. Phys.* **10** 025015

[32] Niu Y, Liang H J, Liu Y, Liu F Y, Ma R and Ding D J 2017 *Chin. Phys. B* **26** 074222

[33] Niu Y, Liu F Y, Liu Y, Liang H J, Yang Y J, Ma R and Ding D J 2017 *Opt. Comm.* **397** 118

[34] Liang H J, Wang Q X, Fan X, Shan L Y, Feng S, Yan B, Ma R and Xu H F 2018 *Chin. J. Chem. Phys.* **31** 471

[35] Miyazaki K, Kaku M, Miyaji G, Abdurrouf A and Faisal F H M 2005 *Phys. Rev. Lett.* **95** 243903

[36] Seideman T and Hamilton E 2005 *Adv. At. Mol. Opt. Phys.* **52** 289

[37] Lock R M, Zhou X, Li W, Murnane M M and Kapteyn H C 2009 *Chem. Phys.* **366** 22

[38] Frisch M J, Trucks G W, Schlegel H B *et al.* 2004 Gaussian 03, Revision E.01 (Wallingford CT: Gaussian Inc.)

[39] Lu T and Chen F 2012 *J. Comput. Chem.* **33** 580

[40] Khan S D, Cheng Y, Möller M, Zhao K, Zhao B, Chini M, Paulus G G and Chang Z 2011 *Appl. Phys. Lett.* **99** 161106

[41] Larsen E W, Carlström S, Lorek E, Heyl C M, Paleček D, Schafer K J, L'Huillier A, Zigmantas D and Mauritsson J 2016 *Sci. Rep.* **6** 39006