

## Research Article

**EFFECT OF THE POTENTIAL WITHIN  
SINGLE-ACTIVE ELECTRON APPROXIMATION  
ON HIGH-ORDER HARMONIC GENERATION FROM CO MOLECULE***Nguyen Thi Hien<sup>1,2,3</sup>, Phan Thi Ngoc Loan<sup>4\*</sup>*<sup>1</sup>*University of Science, Ho Chi Minh City, Vietnam*<sup>2</sup>*Vietnam National University, Ho Chi Minh City, Vietnam*<sup>3</sup>*Tay Nguyen University, Buon Ma Thuot City, Vietnam*<sup>4</sup>*Ho Chi Minh City University of Education, Vietnam*\* *Corresponding author: Phan Thi Ngoc Loan – Email: [loanptn@hcmue.edu.vn](mailto:loanptn@hcmue.edu.vn)**Received: March 11, 2020; Revised: March 23, 2020; Accepted: March 26, 2020***ABSTRACT**

*Constructing the model of single-active electron (SAE) potential for multielectron molecules is essential to investigate the high-order harmonic generation (HHG). Since solving the nonlinear equation to obtain the SAE potential costs computational resource, this potential is constructed after one or two iterations. In this study, we investigate the influence of using the initial SAE potential (the initial wave function is calculated from Gaussian source code), the SAE potential with one iteration (the wave function is obtained after one iteration) on the feature of HHG spectra from CO molecule. We examine the even and odd harmonics, and the even-to-odd ratio of HHG. The results show that, in comparison with the case of using one-iterative SAE, the initial SAE potential causes the missing information at some harmonic orders. However, the choices of SAE potential do not affect the behavior of the even-to-odd ratio in the dependence on the molecular orientation angles. This is an important result allowing us to use the initial SAE in analyzing physical effects.*

**Keywords:** high-order harmonic generation; single-active electron approximation; even-to-odd ratio; asymmetric molecule; core-electron polarization effect

**1. Introduction**

Today, the development of science and technology has promoted discovering new physics phenomena to gain a deeper understanding of atomic and molecular structures. One of them is the high-order harmonic generation (HHG) found in 1987 based on the development of laser technology (Krause, Schafer, & Kulander, 1992; McPherson et al., 1987). HHG is a nonlinear phenomenon occurring when matter (atoms, molecules, solids)

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interacts with an ultrashort ( $\sim$  femtoseconds) and intense ( $>10^{13}$  W/cm<sup>2</sup>) laser pulse. HHG is high-energy photons whose frequency is an integer number of irradiated laser's frequency (Corkum, 1993; Lewenstein, Balcou, Ivanov, L'Huillier, & Corkum, 1994). HHG spectra are characterized by a common feature. Firstly, at low energy, the HHG intensity rapidly drops – called perturbation region. Then, it is followed by a broad plateau region whose intensity is almost unchanged. The plateau is ended by a cutoff, after which the HHG intensity is dramatically depressed (Corkum, 1993; Lewenstein et al., 1994).

There are two main approaches to simulate HHG from atoms, molecules. The first one is using the approximate models such as strong-field approximation (Lewenstein et al., 1994; Zhou, Tong, Zhao, & Lin, 2005), quantum-orbit theory (Milošević, & Becker, 2002), or quantitative rescattering model (Le, Lucchese, Morishita, & Lin, 2009). These models have an advantage in simple analytical formulae; thus, they can be applied for complex systems. The second approach is *ab initio* methods such as the time-dependent density functional theory (Burke, Werschnik, & Gross, 2005), time-dependent Hartree-Fock (Zhang, Yuan, & Zhao, 2014), or numerical method of solving time-dependent Schrödinger equation (TDSE) (Hoang, Zhao, Le, & Le, 2017; Le, Hoang, Tran, & Le, 2018; Zhao, Jin, Le, Jiang, & Lin, 2010). These methods possess higher accuracy but require more computational resources compared to using the approximate models. Therefore, the *ab initio* methods are challenging to apply to multi-electron atoms, molecules. One of the solutions is using the approximate potential with single-active orbital (Zhang et al., 2014), or single-active electron (SAE) (Abu-Samha & Madsen, 2010; Zhao et al., 2010). According to the SAE approximation, only the outermost-shell electron interacts with laser, and it is called the active electron. The remaining electrons, called core-electron, are fixed with the nuclei. Meanwhile, the active electron is affected by the effective field caused by the nuclei and core-electron. The polarization effect of the core-electron occurring when interacting with a laser is called dynamic core-electron polarization (DCeP). The applying of the SAE model in calculating HHG spectra ensures the accuracy of results but saves the computation resource.

To construct SAE potential, the wave function of the multiple atom/molecule is needed. It follows an iteration logic while solving the nonlinear equation: the wave function is required to calculate SAE potential, and conversely, the SAE potential is needed to solve the wave function. The wave function for the first iteration is simulated from the chemical source code, such as Gaussian. Using this wave function, the initial SAE is calculated. Then, this initial SAE potential is used to calculate the new wave function. After that, this wave function is adopted to construct the SAE potential – called SAE potential after the first iteration. We refer it to one-iterative SAE potential. Since solving nonlinear equation by this iteration method takes many computational resources; currently, the SAE potential is restricted to the initial or the one-iterative potentials. Using the initial

SAE, the authors (Hoang et al., 2017; Zhao et al., 2010) have obtained the ionization probability of molecules that is consistent with experiments. However, within this approximation order, the used basis set is Gaussian functions; thus, the SAE potential is less accurate at a large distance (Zhao et al., 2010). Therefore, in recent works (Le et al., 2018; Le, Vu, Ngo, & Le, 2019; Phan, Le, Hoang, & Le, 2019), the authors have exploited the one-iterative SAE potential. Using this potential, the HHG spectra for CO, CO<sub>2</sub> are successfully calculated by the TDSE method. However, there have been no studies focused on the comparison of the accuracy between initial and one-iterative SAE potentials in HHG calculation. Thus, it is necessary to study the accuracy of using SAE potentials.

Recently, there are many studies focused on the HHG spectra from asymmetric molecules, such as CO (Hu, Li, Liu, Li, & Xu, 2017; Le et al., 2018, 2019; Phan et al., 2019; Zhang et al., 2014). Unlike the pure-odd HHG from atoms or symmetric molecules, the HHG from CO contains both odd and even harmonics due to the symmetry breaking of the laser-molecule system (Hu et al., 2017; Phan et al., 2019). One of the quantities characterized the symmetry breaking is the ratio between the intensity of adjacent even and odd harmonics, called even-to-odd ratio. In our recent works (Phan et al., 2019), we have employed the one-iterative SAE potential to simulate odd-even HHG from CO. Using this odd-even HHG spectra, and the even-to-odd ratio as a tool to verify the accuracy of using SAE potential is a possible task needed to be investigated.

The goal of this study is to investigate the influence of using two types of SAE potential – (i) initial and (ii) one-iterative SAE potentials, on the feature even-to-odd ratio and odd-even HHG spectra from CO molecule. We investigate two cases – ignoring and including the DCeP effect. The HHG spectra are calculated by the TDSE method.

## 2. Theoretical background

In this paper, to calculate the HHG spectra, we numerically solve the time-dependent Schrödinger equation (TDSE) in the framework of the SAE approximation for the interaction between the CO molecule and a laser. First, we present the SAE potential model, then followed by a brief description of the TDSE method for calculating HHG.

### 2.1. SAE model

The potential of a multi-electron molecule such as CO is built using the SAE approximation model, which describes the interaction of an active electron interacting with the effective field creating by the nuclei and the remaining electrons. The SAE model has been presented in many references, such as (Abu-Samha, & Madsen, 2010; Zhao et al., 2010). Here, we recall some of the main formulae.

Potential  $V_{SAE}(\mathbf{r})$  includes components

$$V_{SAE}(\mathbf{r}) = V_{en}(\mathbf{r}) + V_{ee}(\mathbf{r}) + V_{ex}(\mathbf{r}), \quad (1)$$

with

$$V_{en}(\mathbf{r}) = -\sum_i^N \frac{Z_i}{|\mathbf{r} - \mathbf{R}_i|} \quad (2)$$

is the electrostatic potential between the active electron and the nuclei, where  $Z_i$  and  $\mathbf{R}_i$  are the charge and position of the  $i$ -nucleus.

$$V_{ee}(\mathbf{r}) = \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \quad (3)$$

is the potential between the active electron and the remaining electrons, where  $\rho(\mathbf{r})$  is the electron density.

The exchange potential  $V_{ex}(\mathbf{r})$  consists of two components

$$V_{ex}(\mathbf{r}) = \alpha V_{ex}^{LDA}(\mathbf{r}) - \gamma V_{ex}^{GC}(\mathbf{r}), \quad (4)$$

where  $V_{ex}^{LDA}(\mathbf{r}) = -\left(\frac{6\rho_\sigma(\mathbf{r})}{\pi}\right)$  is the exchange potential in local density approximation;

and  $V_{ex}^{GC}(\mathbf{r}) = \frac{X(\mathbf{r})^2 \rho_\sigma(\mathbf{r})^{1/3}}{1 + 3\gamma X(\mathbf{r}) \sinh^{-1}[X(\mathbf{r})]}$  is the correction term to ensure the asymptotic

conditions (Abu-Samha & Madsen, 2010; Zhao et al., 2010). Here,  $X(\mathbf{r}) = \left| \frac{\partial \rho_\sigma(\mathbf{r}) / \partial r}{\rho_\sigma(\mathbf{r})^{4/3}} \right|$

depends on the gradient of the electron density that has the same spin  $\rho_\sigma(\mathbf{r})$ .  $\alpha, \gamma$  are two constants that are optimized to obtain the ionizing potential of the molecule coinciding with the experiment.

Notably, in the formulas (3) and (4), there are electron densities  $\rho(\mathbf{r})$  và  $\rho_\sigma(\mathbf{r})$ . To determine these electron densities, we need to determine the wave function of the electron system. In this article, we use two ways to calculate this wave function. (i) One is to use the wave function calculated from the chemistry source code Gaussian 03 with the Hartree-Fock method, aug-cc-pVTZ basis set. (ii) Second, use wave function after one iteration to build SAE potential. Specifically, from the Gaussian wave function, we obtain the initial SAE potential. We then solve the stationary Schrödinger equation of this initial SAE and obtain the wave function. From the new wave function, we recalculate the electron density  $\rho(\mathbf{r})$  and  $\rho_\sigma(\mathbf{r})$ , from that, rebuild the SAE potential. We call this the one-iterative SAE potential. The energy of the  $5\sigma$  state of CO is  $-0.56$  a.u. and  $-0.51$  a.u. for initial and one-iterative SAE potentials.

### 2.2. TDSE method

The time-dependent Schrödinger equation described the interaction of a molecule with a laser field in the atomic unit system has the following form

$$i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = (\hat{H}_0(\mathbf{r}) + \hat{H}_i(\mathbf{r}, t)) \psi(\mathbf{r}, t), \quad (5)$$

where  $\hat{H}_0(\mathbf{r}) = -\frac{\nabla^2}{2} + V_{SAE}(\mathbf{r})$  is the field-free Hamiltonian.  $\hat{H}_i(\mathbf{r}, t) = V_e(\mathbf{r}, t) + V_p(\mathbf{r}, t)$  is the time-dependent Hamiltonian describing the interaction of a molecule with a laser field, in which  $V_e(\mathbf{r}, t) = \mathbf{r} \cdot \mathbf{E}(t)$  presents the interaction between the active electron and the laser.

The potential  $V_p(\mathbf{r}, t) = -\frac{\mathbf{E}(t) \hat{\alpha}_c \mathbf{r}}{r^3}$  exhibits the interaction of the core-electron with the laser field, where  $\hat{\alpha}_c$  is the core-electron polarization tensor, whose parameters for the CO molecule are presented in Ref. (Hoang et al., 2017). In this paper, we consider both cases - ignoring the DCeP effect by neglecting the polarity potential  $V_p(\mathbf{r}, t)$ ; and considering the DCeP effect by including  $V_p(\mathbf{r}, t)$ .

$E(t) = E_0 f(t) \cos \omega t$  is the time-dependent laser electric field, where  $E_0, f(t), \omega$  are respectively the electric amplitude, the envelope function and the carrier frequency of the laser. In this article, we use a 10-cycle laser, which has the trapezoidal envelope with one-cycle turns on, one-cycle turns off. A laser with an intensity of  $1.5 \times 10^{14}$  W/cm<sup>2</sup>, a wavelength of 800 nm, is used throughout the article.

The laser is irradiated so that its electric vector makes with the molecular axis an angle  $\beta$  - called the molecular alignment angle. The system model is shown in Figure 1.

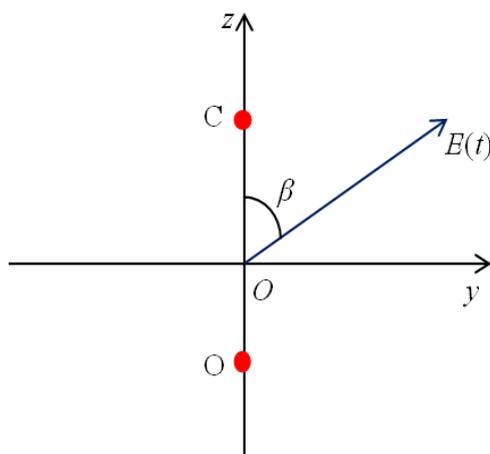


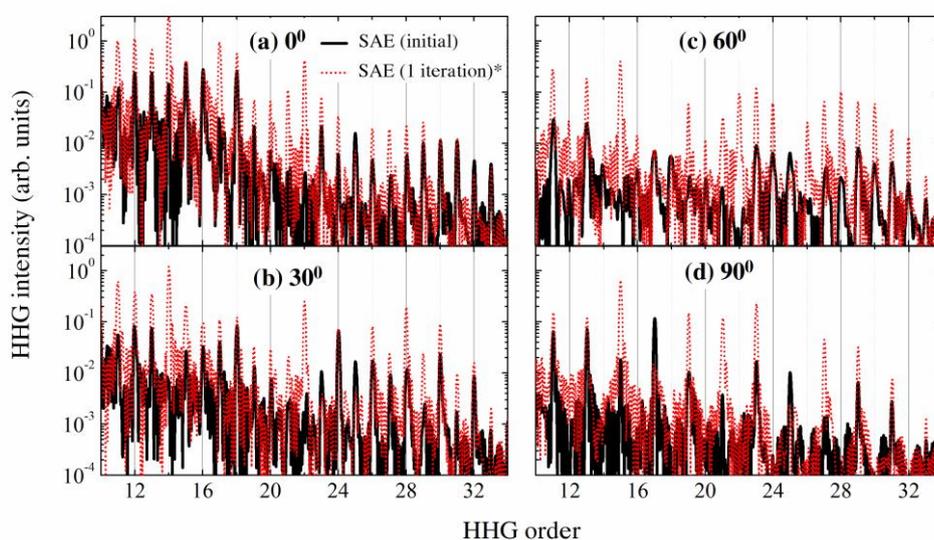
Figure 1. Model of CO molecule interacting with a linearly polarized laser

TDSE equation (5), and HHG spectra are solved by the method stated in the works (Le et al., 2018; Phan et al., 2019). The calculation parameters are given in the Ref. (Phan et al., 2019).

### 3. Results

In this section, we present the HHG spectra from CO molecule calculated by the TDSE method in the framework of SAE approximation in the two cases of using (i) initial; and (ii) one iterative SAE potentials. It should be noted that the HHG for CO within one-iterative SAE potential was published in Ref. (Phan et al., 2019). Here, we reuse these results as a measure of the accuracy of the initial SAE potential. We consider only the HHG with the polarization parallel to the laser electric field and called parallel HHG. The results for HHG with perpendicular polarization are similar.

#### 3.1. Ignoring dynamic core-electron polarization



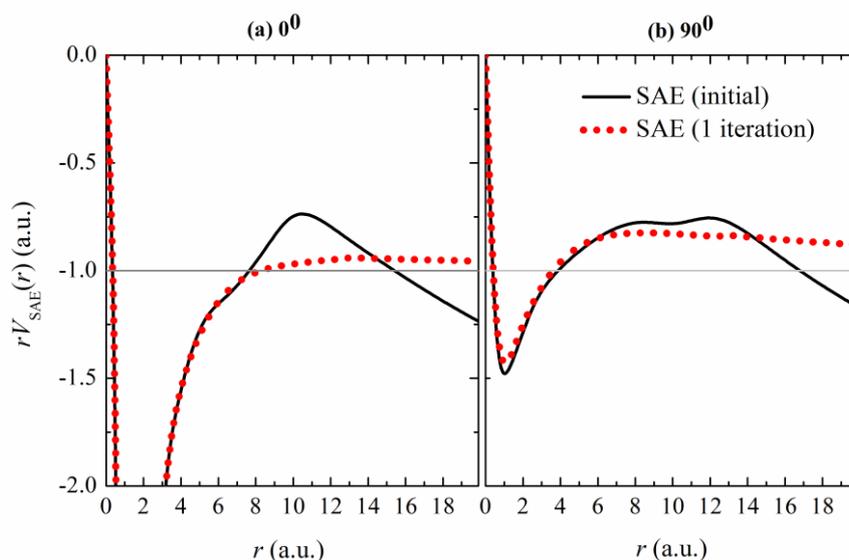
**Figure 2.** The HHG intensity of CO molecule when ignoring the DCEP effect for alignment angles  $0^\circ$  (a),  $30^\circ$  (b),  $60^\circ$  (c), and  $90^\circ$  (d) within the initial, and one-iterative SAE potentials. The laser with an intensity of  $1.5 \cdot 10^{14} \text{ W/cm}^2$ , a wavelength of 800 nm, and a duration of 10 optical cycles is used. \* Results are extracted from (Phan et al., 2019)

First, we investigate the case of ignoring the DCEP effect of CO molecule. Figure 2 presents the HHG spectra from the CO molecule with the initial SAE potential for different alignment angles. The results show that the HHG spectra have a cutoff at 29<sup>th</sup> harmonics. Moreover, the cutoff is almost unchanged with different alignment angles. The cutoff energy is satisfied with the cutoff law according to the three-step model,  $I_p + 3.17U_p$  (Lewenstein et al., 1994), i.e., the 27<sup>th</sup> harmonics. Here,  $I_p$  and  $U_p$  are the ionization potential of CO and the ponderomotive energy of an electron in the laser field. Besides, we pay attention to the odd-even property of the HHG spectra. It is shown that for alignment angles from  $0^\circ$  to  $60^\circ$ , the HHG spectra contain both odd and even harmonics. However,

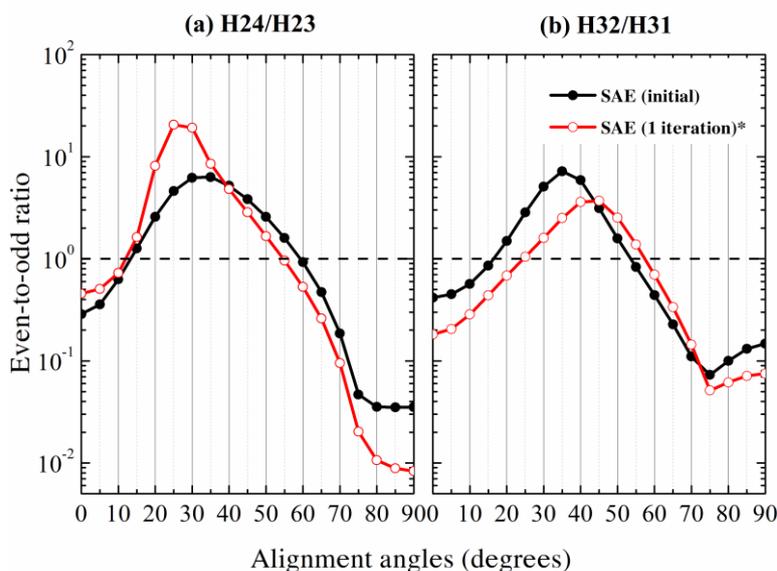
for angles from  $75^\circ$  to  $90^\circ$ , the parallel HHG consists of only odd harmonics. These results are consistent with those of recent works calculated for CO with one-iterative SAE potential (Phan et al., 2019) and full potential (Hu et al., 2017).

To comparison, in Figure 2, we also present the HHG spectra for CO within one-iterative SAE potential (Phan et al., 2019). We find that there is a difference in HHG intensity between the two cases. The one-iterative SAE potential gives the HHG with higher HHG intensity compared to that with the initial SAE potential. This finding can be explained by the fact that the ionization potential of the initial SAE potential is higher than that of the one-iterative one. As a consequence, the ionization probability and the HHG intensity of the initial potential is smaller. Besides, for spectra with the initial SAE potential, its HHG spectra lost the peaks from H19 to H22. We claim that the reason is the inaccuracy of the initial SAE potential in the asymptotic region. The Fig. 3 shows that for  $r > 5$  a.u., the initial SAE potential of CO molecule does not satisfy the asymptotic condition that it reaches  $-1/r$ . However, the one-iterative SAE potential has improved this inaccuracy, resulting in the sufficiency of harmonic orders in HHG spectra.

However, qualitatively, the intensity correlation between the even and odd harmonics in HHG from CO with the initial, and one-iterative SAE potential, are the same. In particular, Fig. 2 shows that for alignment angle  $0^\circ$ , and  $60^\circ$ , the HHG intensity of the even and odd HHG orders is comparable. For  $\beta = 30^\circ$ , for harmonics near the cutoff, the intensity of the even HHG order is more efficient than that of the odd ones. When the laser electric field is perpendicular to the molecular axis, i.e.  $\beta = 90^\circ$ , the HHG spectra contains only odd harmonics.



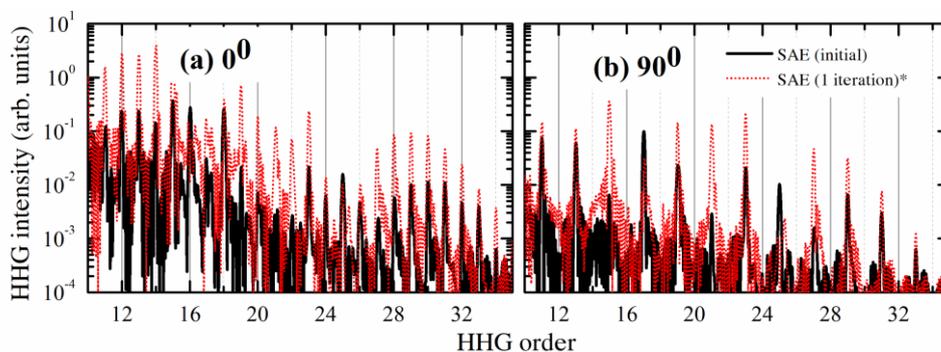
**Figure 3.** The  $rV_{SAE}(r)$  value of the initial and one-iterative SAE potentials of CO molecule with azimuth angle  $0^\circ$  (a), and  $90^\circ$  (b)



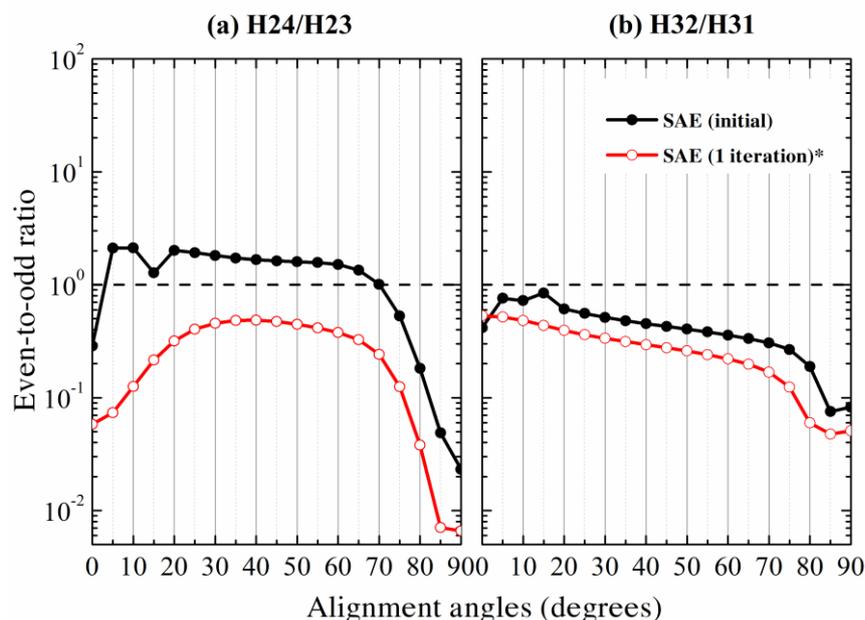
**Figure 4.** The alignment dependence of the even-to-odd ratio of harmonics in the plateau (a), and near cutoff (b) of CO with the initial and one-iterative SAE potentials. \* Results are extracted from (Phan et al., 2019)

To explicit the correlation between the even and odd harmonics, we calculate the ratio between the adjacent even and odd harmonics, and referred to the even-to-odd ratio. It is presented in Fig. 4 as a function of the alignment angle. The results show that, for harmonics in the middle plateau (Fig. 4a), and near cutoff (Fig. 4b), the alignment dependences of even-to-odd ratio for initial and one-iterative SAE potentials are similar. Specifically, for the two potentials, the even-to-odd ratio increases from  $0^\circ$  and reaches a maximum when the alignment angle is in the range  $20^\circ - 50^\circ$ . This means that in this range, the even harmonics are more efficient than the odd ones. After that, with increasing the alignment angle, the even-to-odd ratio is rapidly dropped. From  $\beta = 75^\circ$  to  $\beta = 90^\circ$ , this ratio is slowly changed, and the HHG spectra contain only odd harmonics

**3.2. Considering dynamic core-electron polarization**



**Figure 5.** The same as in Fig. 2, but considering the DCeP effect for CO molecule with alignment angle  $0^\circ$  (a), and  $90^\circ$  (b). \* Results are extracted from (Phan et al., 2019)



**Figure 6.** The same as in Fig. 3, but considering the DCEP effect

To continue, we consider the case of including the DCEP effect of CO molecule. Figure 5 presents the HHG spectra from the CO molecule with alignment angle  $0^\circ$  (Fig. 5a), and  $90^\circ$  (Fig. 5b) for initial and one-iterative SAE potentials. The figure shows that the results are similar to the case of ignoring the DCEP effect. In particular, the HHG for initial SAE potential is more efficient than those for the one-iterative potential. Moreover, the HHG for initial potential loses some harmonics in comparison with the spectra for one-iterative potential.

However, considering the HHG intensity, the correlation between the intensity of even and odd harmonics is similar to the case of ignoring the DCEP effect. Figure 6 presents the alignment dependence of the even-to-odd ratio of HHG spectra from the CO molecule with including the DCEP effect. Similar to the case of ignoring the DCEP presented in Fig. 4, the tendency of the curves for the initial and one-iterative SAE potentials are almost the same. In short, we conclude that, although the inaccuracy of initial SAE potential leading to the missing information of harmonics in HHG, but the correlation between the intensity of even and odd harmonics are not affected.

#### 4. Conclusion

In this paper, by the TDSE method, we have studied the influence of using the SAE potentials constructed from the initial wave function calculated from the Gaussian chemical source code, and the SAE potential with one iteration on the parity property and even-to-odd harmonics ratio of HHG spectra from CO molecule. The results show that

using the initial SAE potential to calculate the HHG results in a loss of information at some HHG orders compared to the case of using the one-iterative SAE potential. However, the initial SAE potential does not affect the alignment dependence of the even-to-odd ratio. The results have been validated for both cases - ignoring and taking into account the DCeP effect. This research can be further extended to other asymmetric molecules such as NO, OCS... to examine the generality of the conclusion.

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## ẢNH HƯỞNG CỦA THỂ NĂNG TRONG GẦN ĐÚNG MỘT ELECTRON HOẠT ĐỘNG LÊN PHỔ SÓNG ĐIỀU HÒA BẬC CAO CỦA PHÂN TỬ CO

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### TÓM TẮT

Xây dựng mô hình thế năng gần đúng một electron (SAE) cho phân tử có nhiều electron rất quan trọng trong nghiên cứu phổ phát xạ sóng điều hòa bậc cao (HHG). Do việc giải phương trình phi tuyến để xác định thế SAE chiếm nguồn tài nguyên tính toán rất lớn, người ta thường chỉ tính đến một hoặc hai vòng lặp. Trong công trình này, chúng tôi nghiên cứu ảnh hưởng của việc sử dụng thế SAE ban đầu (hàm sóng ban đầu tính được từ phần mềm Gaussian) và sau một vòng lặp (hàm sóng thu được sau vòng lặp đầu tiên) lên tính chất phổ HHG của phân tử CO. Chúng tôi xem xét các đặc điểm bậc HHG chẵn, lẻ, và tỉ số giữa cường độ bậc HHG chẵn và lẻ trong phổ HHG. Kết quả cho thấy, sử dụng thế năng SAE ban đầu để tính HHG sẽ cho kết quả bị mất thông tin tại một số bậc HHG so với trường hợp sử dụng thế năng SAE sau một vòng lặp. Tuy nhiên, việc sử dụng thế năng SAE ban đầu không ảnh hưởng đến dáng điệu của đường cong mô tả sự phụ thuộc vào góc định phương của tỉ lệ bậc HHG chẵn-lẻ. Đây là kết quả quan trọng cho phép ta sử dụng thế SAE ban đầu trong phân tích một số hiệu ứng vật lý.

**Từ khóa:** sóng điều hòa bậc cao; gần đúng một electron hoạt động; tỉ số bậc chẵn-lẻ; phân tử bất đối xứng; hiệu ứng phân cực động do electron lõi