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Electrostatic surface guiding of cold polar molecules with a single charged wire*

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This paper proposes a scheme to guide cold polar molecules by using a single charged wire half embanked in an insulating substrate and a homogeneous bias electric field, which is generated by a plate capacitor composed of two infinite parallel metal plates. The spatial distributions of the electrostatic field produced by the combination of the charged wire and the plate capacitor and the corresponding Stark potentials (including dipole forces) for metastable CO molecules are calculated, the relationships between the electric field and the parameters of our charged-wire layout are analysed. It also studies the influences of the insulator on the electric field distribution and the discharge effect. This study shows that the proposed scheme can be used to guide cold polar molecules in the weak-field – seeking states, and to form various molecule-optical elements, such as molecular funnel, molecular beam-splitters and molecule interferometer, even to construct a variety of integrated molecule-optical elements and their molecule chips.

Keywords: cold polar molecules, electrostatic field, Stark effect, molecule-optical elements
PACC: 4110D, 3260S

1. Introduction

In recent years, the successes of laser cooling and trapping of neutral atoms and the realization of Bose–Einstein condensations have resulted in a new interest in cold molecule science. Unfortunately, the technique of laser cooling for neutral atoms seems to meet some unavoidable difficulties in the generation of cold molecules because the neutral molecules have much more complex internal energy structure than that of the atoms. For this reason, one has to develop some new other methods to produce and manipulate cold molecules. Fortunately, thanks to the hard work of many scientists and scholars, some main methods have been developed to produce cold molecules, such as the photon association[1−10] or Feshbach resonance association[11,12] of ultracold atoms, the buffer gas cooling,[13−15] the supersonic molecular beam and its Stark deceleration with time-varying electric field[16−23] as well as the energy low-pass filter based on the electrostatic curved guiding.[24−25]

After the generation of cold molecules, on the other hand, one has carried out some experiments on the manipulation and control of cold molecules, such as the laser deflection and focusing of cold molecules,[26] the refraction of cold molecular beams,[27] the diffraction and interference of cold molecules,[28,29] and the guiding of cold polar molecules in the strong-field-seeking state around the inner electrode of a charged cylindrical capacitor in helical trajectories.[30]

In this paper, we propose a simple method to guide cold polar molecules in the weak-field-seeking state by using a single charged wire and a homogeneous bias electrostatic field, and discuss some potential applications of our guiding scheme in molecule optics. In Section 2, we first introduce our molecular guiding scheme and derive the equations to calculate the electric-field distribution from our wire layout and its Stark potential for cold polar molecules. In Section 3, the spatial distributions of the resulting electric field in free space and the corresponding Stark trapping potentials for cold metastable CO molecules are calculated, the relationships between the electric-field distribution (or Stark trapping potentials) and the parameters of our charged-wire layout are analysed in some details. We also study the influences of the Teflon insulator on the discharge effect and the

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electric field distribution at end of the section. In Section 4, we briefly discuss some potential applications of our guiding scheme in the construction of various molecule-optics elements, such as molecular funnel, molecular beam-splitter and molecule interferometer. The main results and conclusions are summarized in the last section.

2. Guiding scheme and derivation of formulas

Our molecular guiding scheme, as shown in Fig.1, is composed of a single charged cylindrical wire and a charged plate capacitor. The wire with a radius r_0 is half embanked in an insulating substrate with a thickness a, and its applied voltage is u_1. One metal plate of the capacitor is placed underneath the substrate and grounded, the other is a transparent plate with a conducting coat (i.e., a transparent electrode) and placed above the substrate with a distance b, and its applied voltage is u_2. Both the wire and the capacitor are assumed to be infinitely long along the z-direction in our calculation for simplicity. According to the so-called image charge method, we derive an analytic expression to calculate the electric field distribution in free space generated by the combination of the charged cylindrical wire and the charged capacitor as follows:

$$E_x = \frac{C_1}{(1+\varepsilon_{\rm r})}\sum_{n=-\infty}^{\infty}\Big[\frac{x}{[y-2n(a+b)-a_1]^2+x^2} - \frac{x}{[y-2n(a+b)+a_1]+x^2}\Big],$$

$$E_y = \frac{C_1}{(1+\varepsilon_{\rm r})}\sum_{n=-\infty}^{\infty}\Big[\frac{y-2n(a+b)-a_1}{[y-2n(a+b)-a_1]^2+x^2} - \frac{y-2n(a+b)+a_1}{[y-2n(a+b)+a_1]^2+x^2}\Big] + C_2, \qquad (1)$$

where $a_1 = \sqrt{a^2 - r_0^2}$, $\varepsilon_{\rm r}$ is the relative permittivity of the insulating substrate (such as for Teflon substrate, $\varepsilon_{\rm r} = 2.1$, which is used in our following discussion. In our former short letter published in *Chin. Phys. Lett.* (**22** (8) 2005), we did not take the influence of the substrate on the electric field distribution into account, and the formulas given there are valid for $\varepsilon_{\rm r} = 0$ only), and the coefficients C_1, C_2 are determined by the following equation group:

$$\int_0^{a-r}\varepsilon_{\rm r}\Big[\frac{C_1}{(1+\varepsilon_{\rm r})}\sum_{n=-\infty}^{\infty}\Big[\frac{1}{y-2n(a+b)-a_1} - \frac{1}{y-2n(a+b)+a_1}\Big] + \frac{C_2}{\varepsilon_{\rm r}}\Big]{\rm d}y = -u_1,$$

$$\int_{a+r}^{a+b}\Big[\frac{C_1}{(1+\varepsilon_{\rm r})}\sum_{n=-\infty}^{\infty}\Big[\frac{1}{y-2n(a+b)-a_1} - \frac{1}{y-2n(a+b)+a_1}\Big] + C_2\Big]{\rm d}y = u_1 - u_2 \qquad (2)$$

and then we have the total electric field distribution

$$|\boldsymbol{E}(x,y)| = \sqrt{E_x^2(x,y) + E_y^2(x,y)}. \qquad (3)$$

From Eqs.(1)–(3), we can calculate the spatial distribution of the electric field $|\boldsymbol{E}(\boldsymbol{r})|$ of our charged-wire layout and analyse the relationships between the electric field and the parameters of the charged-wire system. The corresponding Stark trapping potential for cold polar molecules and its dipole gradient force can also be calculated and analysed from Eqs.(1)–(3). When a polar molecule with a permanent electric dipole moment (EDM) $\boldsymbol{\mu}$ moves in an inhomogeneous electrostatic field $\boldsymbol{E}(\boldsymbol{r})$, it will experience an interaction of electric dipole force due to the first-order Stark effect. The position-dependent Stark potential for cold polar molecules is given by

$$U_E(\boldsymbol{r}) = -\boldsymbol{\mu}\cdot\boldsymbol{E}(\boldsymbol{r}). \qquad (4)$$

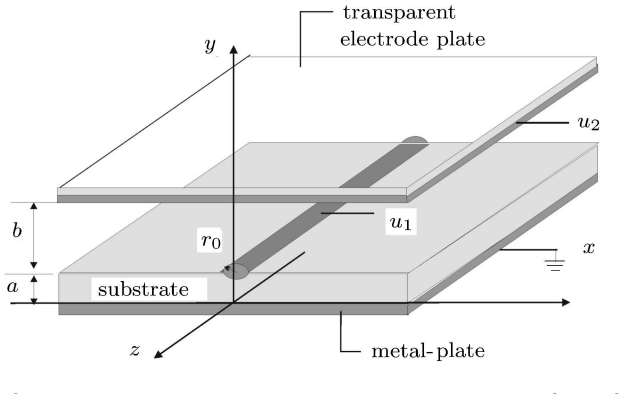


Fig.1. Schematic diagram of molecular electrostatic guiding with the combination of a single cylindrical wire with a radius r_0, the wire is applied by a voltage u_1 on the ceramic substrate with a thickness a, a homogeneous bias field is generated by two infinite parallel metal plates with a distance $(a+b)$ applied a voltage u_2.

When the angle θ between the EDM and the external electric field $\boldsymbol{E}(\boldsymbol{r})$ is fixed, i.e., the molecular motion in the electric field satisfies the condition of adiabatic approximation, we can introduce an effective dipole moment $\mu_{\rm eff} = \mu\langle\cos\theta\rangle$, which depends on the quantum state of the molecule. Here μ is the magnitude of the EDM, and $\langle\cos\theta\rangle$ means the quantum-mechanical expectation value of $\cos\theta$ for a definite

quantum state. Thus, we have

$$U_E(\boldsymbol{r}) = -\mu_{\rm eff} E(\boldsymbol{r}), \tag{5}$$

where $E(r) = |\boldsymbol{E}(\boldsymbol{r})|$.

From Eq.(5), we can see that when the EDM is parallel to the electric field (i.e., $\boldsymbol{\mu}//\boldsymbol{E}$), the interaction potential is attractive, and the molecules in the strong-field-seeking states will be attracted to the maximum place of the electric field, which can be used to guide (or trap) the strong-field-seeking polar molecules. While the EDM is anti-parallel to the electric field (i.e., $\boldsymbol{\mu}//-\boldsymbol{E}$), the potential is repulsive, and the molecules in the weak-field-seeking states will be repelled to the minimum place of the electric field, which can be used to guide (or trap) the weak-field-seeking polar molecules. For a cold metastable CO molecule in the lowest triplet state (the metastable $\alpha^3\Pi$ state), it has a relatively large EDM ($\mu = 1.37$ Debye) and a first-order Stark effect. When the applied electric field is weak, the second-order Stark effect can be neglected, and the trapping potential for cold metastable CO molecules in weak-field-seeking state ($\nu = 0$, $J = 1$, $M\Omega = -1$) takes the approximate form (we neglect the small Lambda splitting of metastable CO for simplicity, which has little influence on our deciding the depth of the potential trap)

$$U_E(\boldsymbol{r}) = -\frac{M\Omega}{J(J+1)}\mu|E(\boldsymbol{r})| = \frac{1}{2}\mu|E(\boldsymbol{r})|, \tag{6}$$

where ν and J are the vibration and rotation quantum numbers of a molecular electronic state respectively, and Ω and M the projections of the total angular momentum $\boldsymbol{J}$ on the molecular axis and the space fixed axis, respectively.

According to Eq.(5), the gradient dipole force experienced by a cold polar molecule in the inhomogeneous electrostatic field $\boldsymbol{E}(\boldsymbol{r})$ is given by

$$\boldsymbol{F}(\boldsymbol{r}) = -\nabla U(\boldsymbol{r}) = \mu_{\rm eff}\nabla|\boldsymbol{E}(\boldsymbol{r})|. \tag{7}$$

Obviously, when $\mu_{\rm eff}$ is negative, the weak-field-seeking molecules will be repelled to the minimum place of the electric field due to the repulsive gradient force $\boldsymbol{F}(\boldsymbol{r})$.

3. Theoretical calculations and analysis

From Eqs.(1)–(3), we can find that the magnitude of the electric field in free space is independent of the coordinate z, so it is only needed to study the electric field distribution in the $x-y$ plane. The contours of the electric field $E(r)$ in the $x-y$ plane generated by our charged-wire system are plotted in Fig.2. It can be seen from Fig.2 that there is a point of zero electric field at the position $(0, y_0)$ above the charged wire, around which the electric field $E(r)$ increases with the radial position r.

In other words, the spatial distribution of the resulting electric field above the surface of the charged wire in Fig.2 looks like a hollow electrostatic tube with a guiding centre $(0, y_0)$, which can be used to guide cold polar molecules in the weak-field-seeking states along the z-direction, which is similar to magnetic guide of cold atoms in the weak-field-seeking states with a single current-carrying wire.[31] In order to ensure that the quantum number M can remain constant during the interaction of the guided molecules with the external electric field, we assume that the motion of the guided cold molecules in the electric field should satisfy the condition of adiabatic approximation. That is, when a cold molecule moves in the external electric field, the internal state of the molecule must follow the change of the electric field without transitions between energy levels.

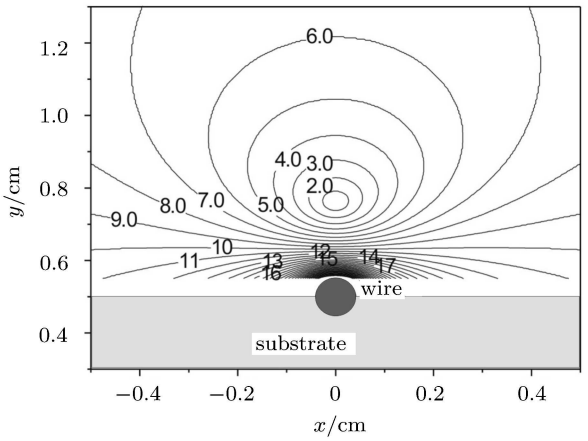


Fig.2. The contours ($x-y$ plane) of the electric field $|E|$ for $a = 5$ mm, $b = 15$ mm, $r_0 = 0.5$ mm, $u_1 = 10$ kV, $u_2 = 15$ kV and $\varepsilon_{\rm r} = 2.1$. The corresponding E-field values are shown in contours, and its unit is kV/cm.

We study the relationships between one-dimensional (1D) distribution of the electric field $E(x, y_0)$ (and $E(0, y)$) and the parameters (u_2, u_1, a, b and r_0) of our guiding system, and obtain some interesting results. The relationships between the corresponding trapping potentials $U(x, y_0)$ (and $U(0, y)$) for metastable CO molecules and the parameters of our

guiding system are also investigated. Here, $E(x, y_0)$ and $U(x, y_0)$ are the 1D distribution of the electric field and its potential distribution for metastable CO molecules along the x-direction at $y = y_0$ respectively; $E(0, y)$ and $U(0, y)$ are those distributions along the y-direction at $x = 0$ respectively.

First, the relationship between the electric field $E(x, y)$ and the voltage u_2 applied on the capacitor is studied, and the results are shown in Fig.3. We can find from Fig.3(a) that the electric field $E(x, y_0)$ is almost linearly changed with the x-coordinate near the guiding centre (somewhat like a quadrupole field), and then gradually increases to its maximum at a large x value. Therefore, the electric field gradient decreases rapidly with the increase of the x-coordinate, and then approached to zero at a large x value. Figure 3(b) presents the relationship between the electric field $E(0, y)$ and the voltage u_2 applied on the capacitor and shows that: (1) there is a point of the zero electric field at the coordinate y_0, which corresponds to the molecular guiding centre $(0, y_0)$ and will be reduced with the increase of the voltage u_2, similar to the case of a magnetic guide for cold atoms by using a single wire;[31] (2) below the guiding centre, the electric field $E(0, y)$ increases rapidly with the reduction of the coordinate y, and reaches the maximum value on the surface of the charged wire, whereas the electric field $E(0, y)$ above the guiding centre y_0 increases gradually with the increase of the coordinate y, and reaches its maximum value near the surface of the upper transparent electrode; (3) the gradient of the electric field $E(0, y)$ below the guiding centre y_0 is far greater than that above the position y_0. According to Eqs.(1)–(3), we derive the relationship between the position y_0 of the guiding centre and the parameters (a, b, r_0, u_1 and u_2) of our guiding system as follows:

$$\frac{C_1}{(1+\varepsilon_{\rm r})}\sum_{n=-\infty}^{\infty}\Big[\frac{1}{y-2n(a+b)-\sqrt{a^2-r_0^2}} - \frac{1}{y-2n(a+b)+\sqrt{a^2-r_0^2}}\Big]+C_2=0, \qquad (8)$$

and study these relationships (see Fig.4). In Eq.(8), C_1, C_2 are the same coefficients as those shown in Eq.(2). We can find from Fig.4 that the position y_0 of the guiding centre reduces with the increase of the voltage u_2 (see Fig.4(a)), and nearly linearly increases with the increase of the voltage u_1 and the geometric parameters a and b (see Figs.4(b), 4(c) and 4(d)), but nonlinearly increases with the increase of the wire radius r_0 (see Fig.4(e)).

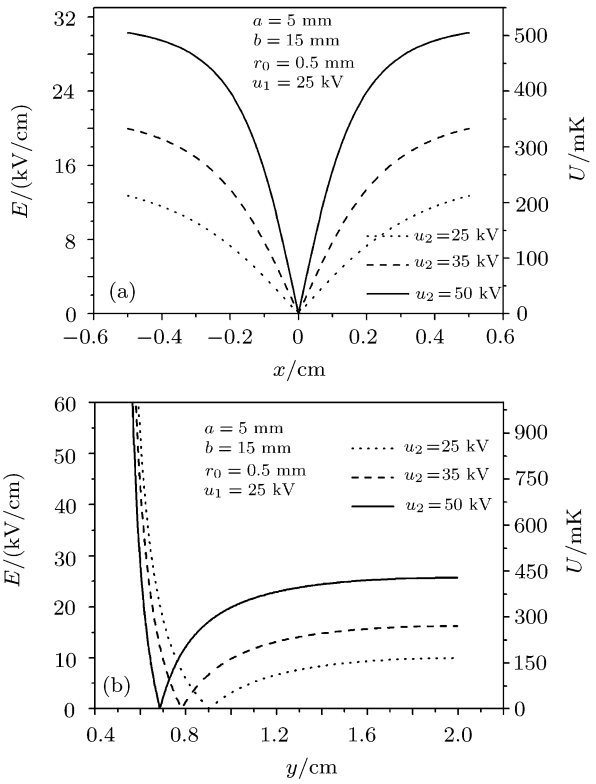


Fig.3. The relationship between the distribution of the E-field and the applied voltage u_2. In which (a) the distribution of $E(x, y)$ at $y = y_0$ and (b) the distribution of $E(x, y)$ at $x = 0$ for $a = 5$ mm, $b = 15$ mm, $r_0 = 0.5$ mm, $u_1 = 25$ kV, and $u_2 = 25$, 35 and 50 kV. The right vertical axis shows the corresponding Stark trapping potential for CO molecules.

It is clear from Fig.3 that for the given parameters a, b, r_0 and u_1, there exits a proper range of the voltage u_2 to form a practical guiding tube above the charged wire. Let us consider a cylindrical guiding tube with a radius $R_0(x, y)$ of 1 mm around the guiding centre $(0, y_0)$ along the z-direction. When $a = 5$ mm, $b = 15$ mm, $r_0 = 0.5$ mm, $u_1 = 25$ kV and $u_2 = 25$ kV−50 kV, and $R_0 = 1$ mm, we have $E(x, y_0)|_{\max} = 4.05$ kV/cm −15.67 kV/cm, and the corresponding trapping potential $U(x, y_0)|_{\max} =$ 67 mK −261 mK. Also, we have $E(0, y)|_{\max}$= 3.22 kV/cm–11.20 kV/cm, and the corresponding potential $U(0, y)|_{\max} = 54$ mK–187 mK. The corresponding coordinate y_0 of the guiding centre is changed from 9.05 mm to 6.86 mm. There are two maximum values in the electric field distribution $E(0, y)$, one is on the surface of the charged wire, and the other is above the zero point y_0 of the electric field, so a smaller one is defined as the effective electric field. In this case, the effective trapping potential $U_E(0, y)_{\rm eff}$

for cold metastable CO molecules is ~ 430 mK when $u_2 = 50$ kV, which is far higher than the transverse temperature (~ 11 mK) of cold polar molecules from the Stark decelerator,[20] and can also be used to guide the supersonic molecular beam with a transverse temperature of ~ 20 mK, which can be estimated by the divergent angle of our supersonic molecular beam. In addition, our study shows that the electric field and the corresponding E-field gradient scale as u_1/s and u_1/s^2 respectively, and the maximum effective trapping potential $U_E(y)_{\text{eff}}$ scales as u_1/s, here s (i.e., $s \equiv y_0$) is defined as the characteristic size of the single-wire guiding system, which is equal to the position y_0 of the guiding centre and can be adjusted by the added voltage u_2.

Next, we study the relations between the electric field E (the trapping potential U) and the geometric parameters (a, b and r_0) of our guiding system, and consider the same cylindrical guiding tube with a radius $R_0(x, y)$ of 1 mm around the guiding centre $(0, y_0)$ along the z-direction, the calculation results are shown in Table 1.

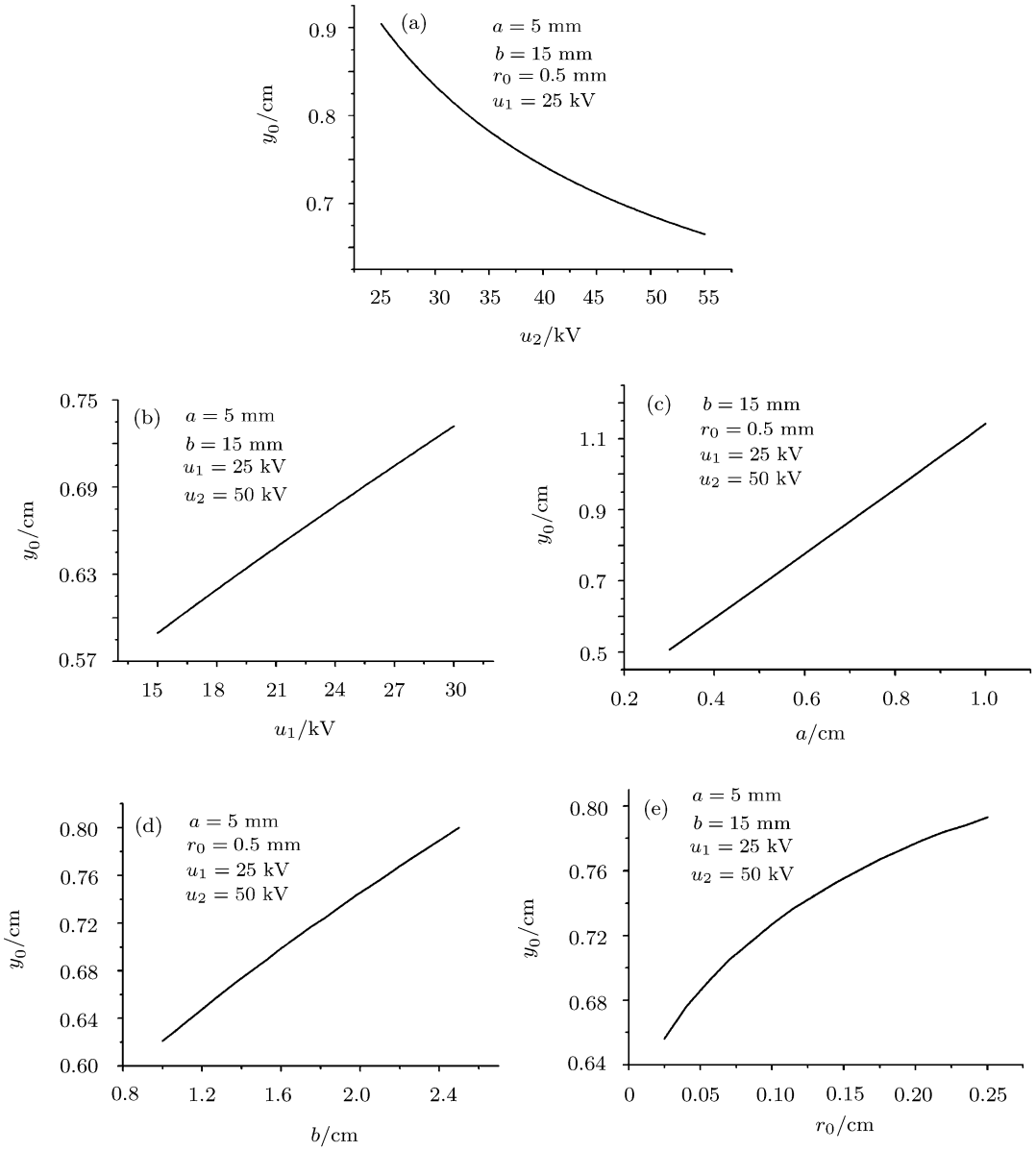


Fig.4. The relationships between the position y_0 of the zero electric field and the parameters u_2, u_1, a, b and r_0 of our guiding system. (a) y_0 versus u_2; (b) y_0 versus u_1; (c) y_0 versus a; (d) y_0 versus b and (e) y_0 versus r_0.

Table 1. The relations between the electric field distribution and geometric parameters when $\varepsilon_r = 2.1$, $u_1 = 10$ kV, $u_2 = 15$ kV and $R_0 = 1$ mm.

Parameter/mm		$E(x,y_0)\|_{max}$/(kV/cm)	$U(x,y_0)\|_{max}$/mK	$E(0,y)\|_{max}$/(kV/cm)	$U(0,y)\|_{max}$/mK	y_0/mm	Given conditions/mm
	3	16.33	272	12.07	201	5.07	($b = 15$ $r_0 = 0.5$)
a	5	15.67	261	11.20	187	6.86	
	7	15.17	252	10.85	180	8.67	
	10	28.10	468	19.80	330	6.20	($a = 5$ $r_0 = 0.5$)
b	15	15.67	261	11.20	187	6.86	
	25	6.96	116	5.45	91	7.99	
	0.25	17.18	286	12.31	205	6.56	($a = 5$ $b = 15$)
r_0	1.25	13.01	216	9.90	165	7.42	
	2.50	9.04	150	7.75	129	7.92	

It is clear from Table 1 that with the increase of parameters a and b, the magnitude of the electric field E (and the corresponding trapping potential U) will decrease, but the influence of the parameter a on E (and U) is smaller, and the influence of the parameter b on E (and U) is greater. Also, we can see from Table 1 that the change of the wire radius r_0 has a relatively remarkable influence on both the electric field E and the corresponding trapping potential U.

Similarly, we also investigate the relationships between the parameters (a, b, r_0 and u_2) and the dipole gradient forces $F(x,y_0)$, $F(0,y)$ experienced by metastable CO molecules, and find that when the voltages u_1 and u_2 are given, the smaller the thickness a and the distance b or the radius r_0 are, the stronger the electric field gradient force is. Moreover, the gradient force of the electric field in the x direction is greater than that in the y direction, as shown in Fig.3. Therefore, in the analysis of the interaction of the guided molecules with the electric field, we only need in fact to consider the distributions of the electric field, trapping potential and its gradient force in the y direction, that is, $E(0,y)$, $U(0,y)$ and $F(0,y) = \mu_{\rm eff}\nabla|E(0,y)|$. When $a = 5$ mm, $b = 15$ mm, $r_0 = 0.5$ mm, $u_1 = 25$ kV and $u_2 = 50$ kV and below the guiding centre $(0,y_0)$, we obtain $F(0,y)|_{\rm min} \geq 7.99\times10^{-23}$ N, which is about 172 times the gravity force exerted on metastable CO molecules. This shows that $F(0,y)$ is strong enough to counteract the action of the gravity force on the guided molecules.

From the above theoretical analysis, we know that for the appropriately applied voltages u_1 and u_2, the smaller the geometric parameters (a, b or r_0) of our guiding system are, the tighter the transverse confinement for the guided cold molecules will be. For instance, when $a = 5$ mm, $b = 10$ mm, $r_0 = 0.5$ mm, $u_1 = 30$ kV and $u_2 = 30 - 50$ kV, the distributions of the resulting electric field and its trapping potentials for metastable CO molecules in the x and y directions are shown in Fig.5.

When $u_2 = 50$ kV, we can see from Fig.5 that the maximum effective electric field $E(0,y)$ is ∼33 kV/cm, and the corresponding maximum effective trapping potential is −550 mK, which can be used to guide a cold molecular beam with a transverse temperature of −0.5 K. Practically, however, we have to carefully choose the geometric parameters (a, b or r_0) so as to avoid the occurrence of discharges.

We also study the influences of the Teflon insulator (with a relative dielectric constant ε_r of 2.1 and a dielectric strength of 60 kV/mm[32]) on the discharge effect and the electric field distribution, and find that when $a = 5$ mm, $b = 10$ mm, $r_0 = 0.5$ mm, $u_1 = 30$ kV and $u_2 = 50$ kV, the maximum electric field near the wire surface is ∼ 150 kV/cm, which is far lower than that (600kV/cm) resulted in discharge. Also, without the Teflon insulator, the maximum effective electric field $E(0,y)$ increases from ∼ 33 kV/cm to ∼37 kV/cm, while the maximum electric field near the wire surface increases to ∼295 kV/cm. This shows that the presence of the isolator can greatly reduce the maximum electric field near the wire surface (by a factor of close to $\sim 1/\varepsilon_r$), but does not seriously influence on the shape of the electrostatic guide tube and its well depth, which depends strongly on the magnitude of the homogeneous bias field. Thus, the presence of the isolator reduces greatly the likelihood of a discharge to occur. In addition, when $a = 5$ mm, $b = 10$ mm, $r_0 = 0.5$ mm, for low values $u_1 = 3$ kV and $u_2 = 4-5$ kV, the effective trapping potential for metastable CO molecules is $39-55$ mK, which is high enough to guide cold polar molecules with a transverse temperature (∼11 mK) from the Stark decelerator,[20] and a transparent electrode with a high voltage of $3-4$ kV may be available.

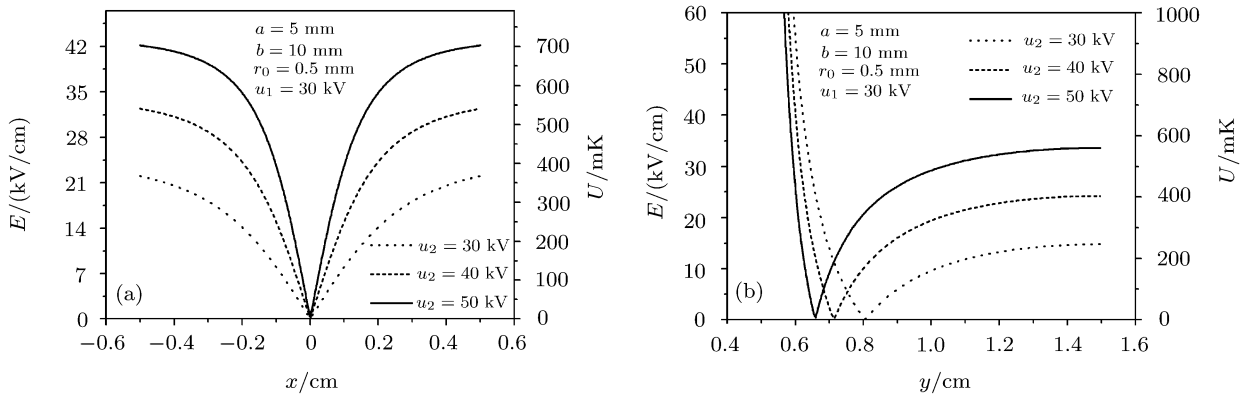


Fig.5. The relationship between the distribution of the E-field and the applied voltage u_2. In which (a) the distribution of $E(x, y)$ at $y = y_0$ and (b) the distribution of $E(x, y)$ at $x = 0$ for $a = 5$ mm, $b = 10$ mm, $r_0 = 0.5$ mm, $u_1 = 30$ kV, and $u_2 = 30$, 40 and 50 kV. The right vertical axis shows the corresponding Stark trapping potential for CO molecules.

4. Potential applications

Molecular funnels, molecular beam-splitters and molecule interferometers and so on are basic molecule-optical elements, which have wide and important applications in the experiments using cold molecules or cold molecular beam. Therefore, the design of various molecule-optical elements is one of the very interesting subjects in the field of molecule optics. Next we will show a few designs of molecule-optical elements and discuss some potential applications of our guiding scheme in molecule optics.

4.1. Molecular funnel

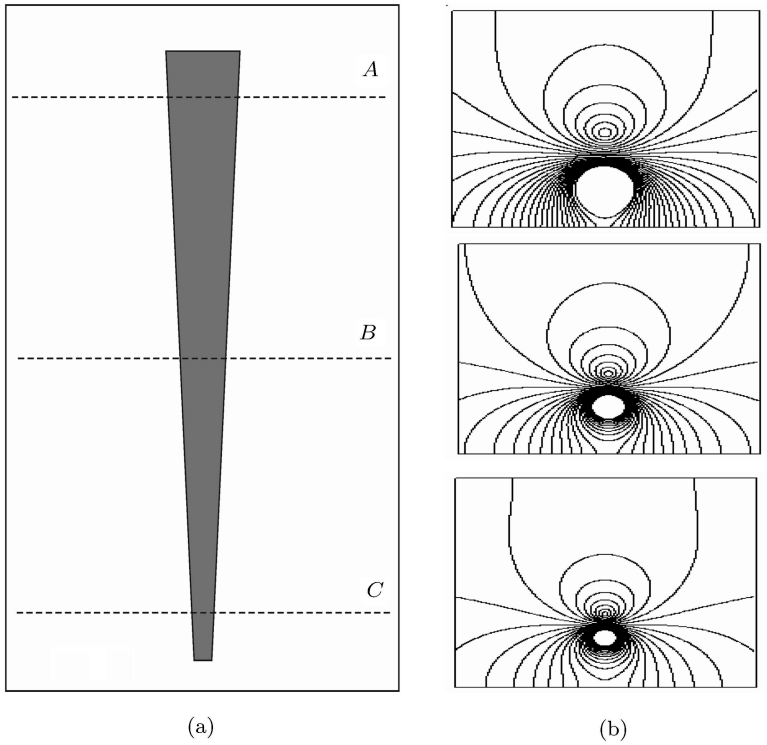


Fig.6. (a) Layout of the molecular funnel based on our guiding scheme (2D vertical view on the $x - z$ plane), and (b) the corresponding contours of the electric field or potential on the $x - y$ plane. Contours are drawn at an interval of 1 kV/cm (i.e. 0.1 kV/mm) and the first contour shows 1 kV/cm with blank circles corresponding to the positions of the charged-wire.

We can find from Table 1 that for the given parameters a, b, u_1 and u_2, the radius of the identical E-field contour will be gradually increased with the increase of the wire radius r_0, which can be used to form a molecular funnel, as shown in Fig.6. Here Fig.6(a) is the two-dimensional (2D) vertical view of the molecular funnel on the $x-z$ plane, and Fig.6(b) depicts the corresponding E-field contours on the $x-y$ plane or the molecular funnel potentials at the different $x-y$ planes A, B and C, respectively. It is clear from Fig.6 that the radius of the E-field contour with an identical magnitude is reduced with the reduction of the wire radius r_0, which likes a funnel and can be used to load a cold polar molecular beam into our single-wire guiding potential.

4.2. Molecular beam-splitter

The simplest molecular beam splitter (MBS) is a Y-shaped one with one input arm and two output arms, which can be formed by a Y-shaped charged-wire guide. Figure 7(a) is the 2D vertical view of our MBS, and Fig.7(b) shows the corresponding E-field contours or Y-shaped molecular guiding potential. It can be seen from Fig.7(a) that when the voltages u_1 and u_2 are applied to our Y-shaped wire system, a single guiding channel will be split into two guiding ones. So ultracold polar molecules will be guided in the input arm, and the molecular wave function can be split after the splitting point of the Y-beam splitting potential, and then they will be guided in both output arms. Since the Y-shaped beam splitting potential is completely symmetric with respect to its input guide, it can be used to realize coherent splitting for many waveguiding modes, which is similar to the case of Y-shaped atomic beam splitter.[33,34] Though the forward velocity of the molecular beam does not play an important role in the guiding, it is different for beam splitters. This is because the maximum splitting angle of the beam splitter will be limited by the forward velocity of the guided molecular beam.

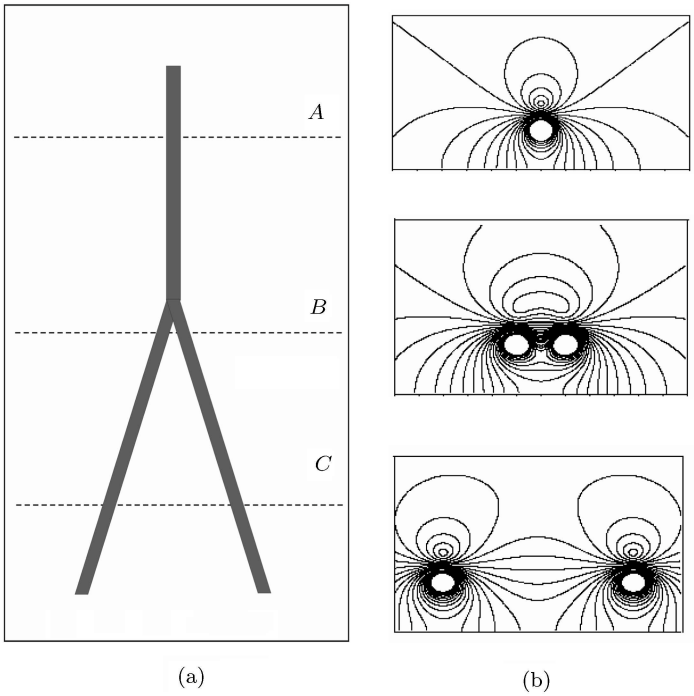


Fig.7. (a) Layout of the Y-shaped molecular beam-splitter (2D vertical view on the $x-z$ plane), and (b) the corresponding contours of the electric field or potential on the $x-y$ plane. Contours are drawn at an interval of 1 kV/cm (beginning at 1 kV/cm) with blank circles corresponding to the positions of the charged-wire.

Similarly, an X-shaped beam splitter with two input arms and two output arms can be formed by using an X-shaped charged-wire system, which is shown in Fig.8. The symmetry of the Y-beam splitter with respect to the input guide, however, is broken and it will be much harder to realize coherent splitting for many waveguiding modes at the same time, which is similar to the case of two-wire X-beam splitter for ultracold atoms.[33] If an X-shaped beam splitter is extended in one- or two-dimensional case, a 1D or 2D quantum network with ultracold molecules will be formed.

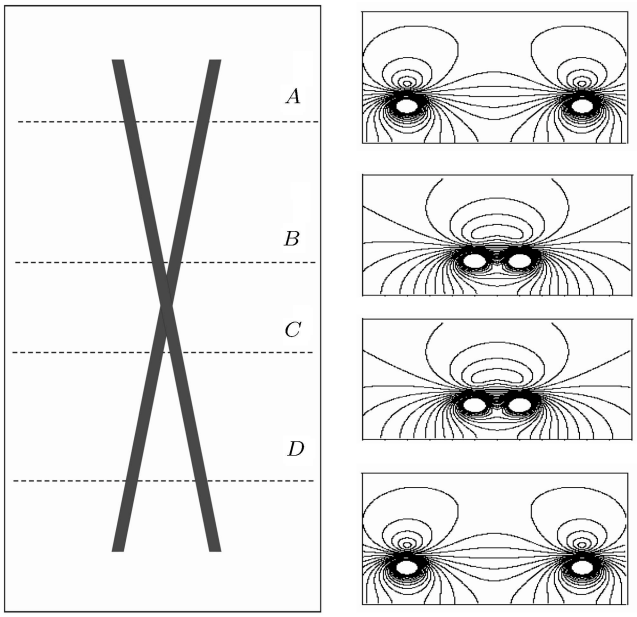


Fig.8. (a) Layout of the X-shaped molecular beam-splitter (2D vertical view on the $x-z$ plane), and (b) the corresponding contours of the electric field or potential on the $x-y$ plane. Contours are drawn at an interval of 1 kV/cm, starting from 1 kV/cm with blank circles corresponding to the positions of the charged-wire.

4.3. Molecule interferometer

When two Y-shaped beam splitters with coherent splitting are connected by their Y-shaped forks, as shown in Fig.9, a molecule interferometer will be constructed. Since the two Y-beam splitting potentials are completely symmetric, the coherent splitting at the first splitting point and coherent superposition at the second converging point, and coherent propagation between two splitting points (in two guiding channels) for many waveguiding modes can be ensured. Obviously, this configuration can be used to realize a superposition of molecular internal states and applied in many experiments on molecular interferometry, which is similar to the case of a multimode interferometer based on wire-guided matter waves.[33,35]

Next, we will briefly discuss the possible loading of cold molecules from a molecular beam into our guide. The above analysis and discussion tell us that, in order to obtain a high transversely trapping potential for the guided molecules, the thickness a, distance b and the wire radius r_0 should be chosen as small as possible for the given appropriate voltages u_1 and u_2. In this case, a proper molecular funnel as shown in Fig.6 can be used to load cold molecules from a Stark-decelerated molecular beam (even a supersonic molecular beam) into our single-wire guiding system, even into our Y-shaped MBS and its molecule interferometer. In addition, if an effusive molecular beam with room temperature is load into our single-wire bent guiding by using a suitable molecular funnel,

a colder CW molecular beam will be generated by using our S-shaped, single-wire bent guiding system (as a low-pass energy filter), which is similar to the experiment of Rempe's group.[24]

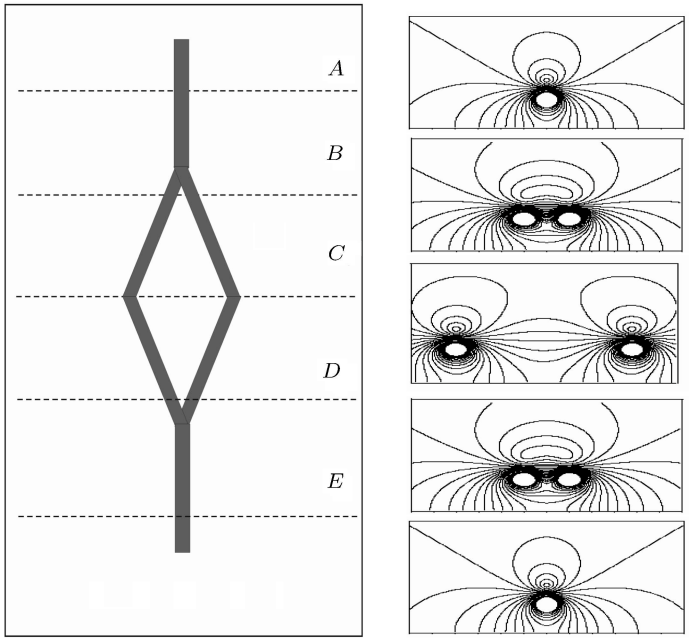


Fig.9. (a) Layout of the molecule interferometer (2D vertical view on the $x-z$ plane), and (b) the corresponding contours of the electric field or potential on the $x-y$ plane. Contours are drawn at an interval of 1 kV/cm, and the first contour indicates 1 kV/cm with blank circles corresponding to the positions of the charged-wire.

5. Conclusions

We have proposed a molecular guiding scheme based on the interaction of an electric dipole moment of the guided molecule with an electric field generated by a single charged wire with a high voltage u_1 on the substrate and a homogeneous bias field, which is generated by an infinite plate capacitor with a high voltage u_2. We have calculated the contours of the electric field, the transverse trapping potential and gradient force for the guided metastable CO molecules, and analysed the relationships between the resulting electric field (including the Stark potential) and the parameters of our guiding layout as well. Our study shows that there is a point of the zero electric field at the position $(0, y_0)$, and the electric field increases rapidly with the increase of the radial distance $r(x, y)$ away from the guiding centre $(0, y_0)$. This looks like a hollow electrostatic tube with an axis of the zero E-field along the z-direction, and then the cold, weak-field-seeking polar molecules moving in the electrostatic tube will be reflected by the repulsive dipole force from the tube. So our charged-wire scheme can be used to guide cold polar molecules along the wire direction (i.e., the z-direction). Since our molecular guiding scheme is a side guiding one for the weak-field-seeking molecules, not a Kepler guiding one for the strong-field-seeking molecules,[36] a higher guiding efficiency (such as more than $\sim 50\%$, even 80–90%) may be readily obtained after considering other loss mechanisms of the guided molecules, such as the collision loss from the background hot molecules, and so on.

Moreover, our electrostatic guide for cold polar molecules has some interesting characteristics, such as the position of the guiding centre, the potential-well depth and its dipole gradient force are not only dependent on the applied voltage u_1 and u_2, but also on the geometric parameters (a, b and r_0) of the charged-wire layout. So we have multiple freedoms to manip-

ulate and control the motion of cold molecules in the guiding tube. In particular, our single-wire guide can be conveniently used to construct various molecule-optical elements, such as molecular funnel, Y- or X-shaped molecular beam-splitters and molecule interferometer, and to generate CW cold molecular beam, even to form a variety of integrated molecule-optical elements on the surface of a substrate and novel molecular chips, and the relative experiments will be considered in our next study.

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