Electrostatic surface guiding of cold polar molecules with double charged wires

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We propose a novel scheme to guide cold polar molecules on the surface of an insulating substrate (i.e., a chip) using a static electric field generated by the combination of a pair of parallel charged wires and a grounded metal plate. We calculate the spatial distributions of the electric fields from the above charged-wire layout and their Stark potentials for cold CO molecules, and analyze the relationships between the electric field and the parameters of the charged-wire layout. The result shows that this charged-wire scheme can be used to guide cold polar molecules in the weak-field-seeking state and to form various molecule-optical elements, even to realize a single-mode molecular waveguide on a molecule chip under certain conditions.

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In recent years, there is a special interest in cold or ultracold molecules, as they are promising for molecular precision spectroscopy and measurements[1,2], studies of cold molecular collisions[3−8], quantum information processing[9], and so on. Some methods, such as Buffer-gas cooling of the paramagnetic molecules[10], photoassociation[11] or Feshbach resonance[12] of precooled atoms in a magneto-optical trap, Stark-slowing in time-varying electric field[13], as well as velocity filter based on the electrostatic curved guiding[14,15], have been developed to create cold or ultracold molecules. On the other hand, manipulating and controlling cold molecules using some new techniques have been experimentally demonstrated. In 2000, Loesch *et al.* demonstrated the Keppler-type electrostatic guiding of polar molecules (NaCl, NaBr, and NaI) in strong-field-seeking state[16]. Since the molecules in the injected polar molecule beam that can satisfy the Keppler motion orbit are very less, the guiding efficiency of strong-field-seeking molecules is very low. For example, the maximum guiding efficiency of NaBr molecules is only $\sim 0.12\%$. Recently, an electrostatic bend guiding technique was used to produce a continuous cold polar molecular beam (H_2CO, ND_3) in the weak- or strong-field-seeking states by using a two-dimensional (2D) quadrupole electrostatic or time-varying electric field, which is generated by the four identical bend charged electrodes[14,15]. However, these guiding schemes cannot be used to realize surface guiding of cold molecules on a substrate (i.e., a chip). So it would be interesting and worthwhile to find a high-efficient guiding scheme and realize an electrostatic surface guiding of cold polar molecules in the weak-field-seeking state on the molecular chip.

In this paper, we propose a novel and simple scheme to guide cold polar molecule on the surface of an insulating substrate (i.e., a chip) using a hollow electrostatic field generated by the combination of a pair of parallel charged wires and a grounded metal plate, and discuss some potential applications of our guiding scheme in molecule optics.

The molecular guiding scheme, shown in Fig. 1, consists of two parallel charged wires (i.e., two cylindrical stainless steel rods) on the surfaces of an insulating substrate and a grounded metal plate. Here the radius of the wire is r_0, the space between centers of two wires is $2a$, and the distance from the wire center to the grounded metal plate is b, the relative dielectric constant of the selected insulating material is ε_r. A high power supplied with a voltage $+U$ is applied to both two wires and used to produce a hollow quadrupole electrostatic-field distribution with a central minimum, so as to realize the electrostatic guiding of cold polar molecules in the weak-field-seeking state on the substrate surface. We assume that the charged wires are infinitely long in the z-direction, according to the Poisson equation and method of images (i.e., the image charge method), the x- and y-directional distribution of the electric field generated by the charged-wire system can be calculated by

$$\begin{aligned}\mathbf{E} &= E_x\,\mathbf{i} + E_y\,\mathbf{j} \\ &= \frac{U}{C}\left[\frac{x-a_1}{(x-a_1)^2+(y-b_1)^2} - \frac{x-a_1}{(x-a_1)^2+(y-b_2)^2}\right. \\ &\left. + \frac{x-a_2}{(x-a_2)^2+(y-b_1)^2} - \frac{x-a_2}{(x-a_2)^2+(y-b_2)^2}\right]\frac{2}{\varepsilon_r+1}\mathbf{i} \\ &+ \frac{U}{C}\left[\frac{y-b_1}{(x-a_1)^2+(y-b_1)^2} - \frac{y-b_1}{(x-a_1)^2+(y-b_2)^2}\right. \\ &\left. + \frac{y-b_2}{(x-a_2)^2+(y-b_1)^2} - \frac{y-b_2}{(x-a_2)^2+(y-b_2)^2}\right]\frac{2}{\varepsilon_r+1}\mathbf{j},\end{aligned} \tag{1}$$

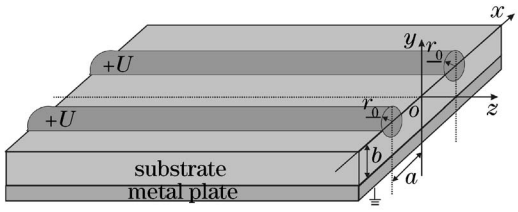

Fig. 1. Schematic diagram of molecular surface electrostatic guiding.

where the coefficients C is determined by

$$\frac{2C}{1+\varepsilon_{\rm r}}\int_{-r_0}^{-b}\left[\frac{y-b_1}{(a-a_1)^2+(y-b_1)^2}-\frac{y-b_1}{(a-a_1)^2+(y-b_2)^2}\right]{\rm d}y + \int_{-r_0}^{-b}\left[\frac{y-b_2}{(a-a_2)^2+(y-b_1)^2}-\frac{y-b_2}{(a-a_2)^2+(y-b_2)^2}\right]{\rm d}y = U, \tag{2}$$

here

$$a_1=\sqrt{a^2+r_0^2}-(\sqrt{a^2+b^2}-\sqrt{a^2+b^2-r_0^2})\frac{a}{\sqrt{a^2+b^2}},\quad a_2=-a_1, \tag{3}$$

$$b_1=-[(b-\sqrt{b^2-r_0^2})+(\sqrt{a^2+b^2}-\sqrt{a^2+b^2-r_0^2})\frac{a}{\sqrt{a^2+b^2}}],\quad b_2=-2b-b_1, \tag{4}$$

then the total electric field distribution is given by

$$|\mathbf{E}(x,y)|=\sqrt{E_x^2(x,y)+E_y^2(x,y)}. \tag{5}$$

From Eqs. (1)—(5), we can calculate the spatial distribution of the electric field $|E|$ from the charged wires layout, and analyze the relationship between the electric field distribution $|E|$ and the parameters (a, b, and r_0) of the guiding system. The corresponding Stark trapping potential for cold polar molecules and its dipole gradient force can also be calculated and analyzed. When a polar molecule with a permanent electric dipole moment (EDM) moves in an inhomogeneous electrostatic field, due to the first-order Stark effect, it will feel a dipole gradient force, and the interacting Stark potential for cold polar molecules can be given by

$$W_{\rm Stark}=-\boldsymbol{\mu}\cdot\mathbf{E}(r). \tag{6}$$

From it, we can see that when $\boldsymbol{\mu}\cdot\mathbf{E}(r)$ is positive (i.e., $\boldsymbol{\mu}//\mathbf{E}(r)$), the Stark potential is attractive, and the molecule in the strong-field-seeking state will be attracted to the maximum of the electrostatic field, which can be used to guide the strong-field-seeking molecules around the charged wire[16]. When $\boldsymbol{\mu}\cdot\mathbf{E}(r)$ is negative (i.e., $\boldsymbol{\mu}//-\mathbf{E}(r)$), the potential is repulsive, and the molecules in the weak-field-seeking state will be repulsed to the minimum of the electric field, which can be used to realize the electrostatic guiding (i.e., 2D trapping) of cold weak-field-seeking molecules[14,15]. For a CO molecule in the metastable $a^3\Pi$ ($J=1$, $M\Omega=-1$) state, it has a relatively large EDM with 4.6×10^{-30} C·m and a strong first-order Stark effect, and the confining potential for the CO molecule can be given by

$$W_{\rm Stark}(\mathbf{r})=-\frac{M\Omega}{J(J+1)}\mu|E(\mathbf{r})|. \tag{7}$$

From Eqs. (1)—(5), we calculate the contours of the electric field $|\mathbf{E}(r)|$ generated by the charged-wire layout, and the result is shown in Fig. 2. We can see that there is a point of zero electric field at the y-axis, and its coordinate position (the guiding center) is at (0, y_0), which is like a hollow electrostatic tube with a point of $|\mathbf{E}(r)|=0$ at the position (0, y_0) and can be used to guide cold polar molecules in the weak-field-seeking state along the z-direction. As we all know that when the guided cold molecules move near the point of zero electric field, they may be lost by Majorana transitions. In order to eliminate this molecular loss, we can add a small bias field E_0 along the guiding axis (i.e. the z-direction) to provide a quantized axis for the guided molecules. According to Eq. (1)—(5), we also can derive the relationship between the position y_0 of the guiding center (zero electric field) and the parameters (a, b, and r_0) of our guiding layout as follows

$$y_0=-b+\left\{\left[\sqrt{a^2+r_0^2}+a\left(-1+\frac{\sqrt{a^2+b^2-r_0^2}}{\sqrt{a^2+b^2}}\right)\right]^2 + \left[\sqrt{b^2-r_0^2}+b\left(-1+\frac{\sqrt{a^2+b^2-r_0^2}}{\sqrt{a^2+b^2}}\right)\right]^2\right\}^{\frac{1}{2}}. \tag{8}$$

When teflon is used as an insulating dielectric substrate, the relative dielectric constant $\varepsilon_{\rm r}$ and dielectric strength of the insulating material are 2.1 and 60 kV/mm, respectively[17]. We study the relationships between the distribution of the electric field ($E(x)|_{y=y_0}$ or $E(y)|_{x=0}$) and the parameters (a, b, and r_0) of the charged-wire layout, and also analyze the relationship between the corresponding Stark potential for CO molecules ($W(x)_{\rm Stark}|_{y=y_0}$ or $W(y)_{\rm Stark}|_{x=0}$) and the parameters of the charged-wire system. From Eqs. (1)—(5) and (7), we calculate the distributions of the electric field and its trapping potential in the x and y-direction, and results are shown in Fig. 3. We can see from Fig. 3(a)

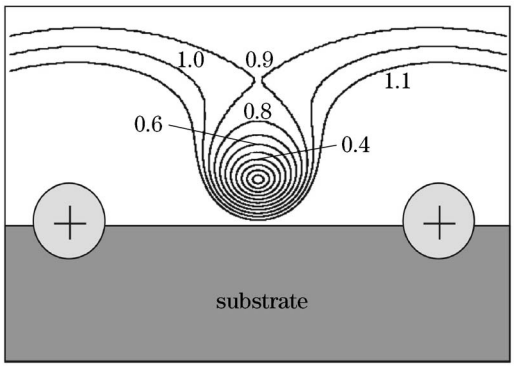

Fig. 2. The contours (x-y plane) of the electric field for a = 3.0 mm, b = 4.0mm, U = 15 kV, and r_0 = 1.0 mm. The electric values are shown in the contours, and its unit is 0.5 kV/cm. The crisscross stands for the positions of two charged wires.

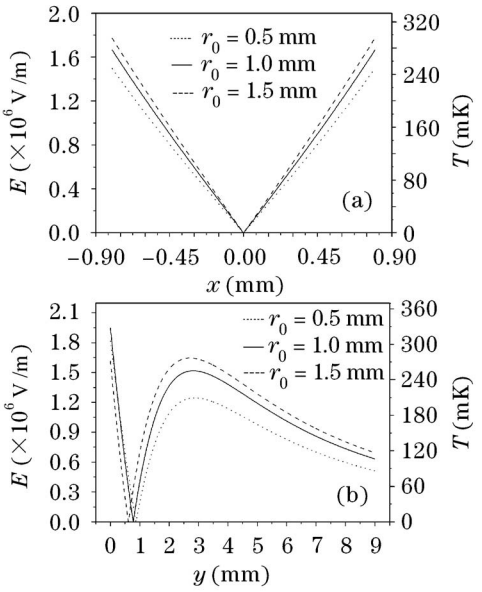

Fig. 3. The relationships of the radius r_0 to (a) the electric field $E(x)$ at $y = y_0$ (the corresponding trapping potential) and (b) $E(y)$ at $x = 0$ for $a = 2.0$ mm, $b = 3.0$ mm, and $U = 30$ kV.

that the larger the radius r_0 is, the larger the gradient of the electric field is, and the higher the maximum electric field $E(x)_{\max}$ (or the Stark potential $W(x)_{\text{Stark}}$) in the x-direction. We also find that the electric field $E(x)$ at $y = y_0$ is almost linearly changed with the x coordinate near the guiding center, it is somewhat like a quadrupole field. Figure 3(b) indicates that 1) with the increase of the radius r_0, the position y_0 of zero electric field will be lowered, but the gradient of the electric field $E(y)$ will be increased; 2) there are two maximum values in the electric field distribution $E(y)$, one is at the surface of the metal plate, and the other is above the zero point y_0 of the electric field, which can be regarded as the maximum effective trapping potential for cold molecules; 3) when $a = 2.0$ mm, $b = 3.0$ mm, $U = 30$ kV, and $r_0 = 1.5$ mm, we obtain the maximum electric field $E(x)_{\max} \approx 1.8 \times 10^6$ V/m and the corresponding trapping potential $W(x)_{\text{Stark}} \approx 300$ mK at $y = y_0$, and the maximum effective electric field $E(y)_{\max} \approx 1.5 \times 10^6$ V/m and the maximum effective trapping potential $W(y)_{\text{Stark}} \approx 250$ mK at $x = 0$. The trapping potential can also be used to guide the supersonic molecular beam with a transverse temperature of about 20 mK, which can be estimated by the divergent angle of the supersonic molecular beam, and similar to one (11 mK) of the Stark-decelerated molecular beam[18].

The result shows that the higher the applied voltage U is, the smaller the geometric parameters (a and b) are, the larger the wire radius r_0 is, the higher the Stark trapping potential for cold molecules is, and the transverse confinement for cold molecules will be more tight, then the average diameter (i.e., the mean transverse moving range) of the guided cold molecules in the hollow electrostatic tube generated by this double-wire layout will become very small. In particular, when this diameter is closed to the mean wavelength of de Broglie wavelength $\lambda = \sqrt{2\pi\hbar^2/(mkT)}$ of cold molecules, it seems possible to realize a single-mode molecular waveguide. Therefore, our electrostatic guiding scheme can be used not only to realize the surface guide or single-mode waveguide of cold polar molecules on a chip, but also to construct various molecule-optical elements, such as molecular funnel, molecular beam-splitter, molecular interferometer, as well as to develop some integrated molecule chips.

Our parallel wires can be fabricated on the insulating substrate by using standard microfabrication techniques (such as photolithography and electroplating)[19]. In consideration of the discharging effect between the positive and negative poles, the distance b between the centers of the charged wires and the grounded plate cannot be taken small too much. When $b = 3.0$ mm, $r_0 = 1.5$ mm, and $U = 30$ kV, the average strength of electric field between the charged wires and the grounded plate is 20 kV/mm, which is less than dielectric strength of the insulating material teflon of 60 kV/mm[17]. So the discharging effect problem of the charged wires on the substrate can be solved well by the selected suitable insulating material.

In summary, we propose a novel scheme to realize electrostatic surface guiding of cold polar molecules on the surface of an insulating substrate (i.e., a chip) using a static electric field generated by the combination of a pair of parallel charged wires and a grounded metal plate, calculate the corresponding electric field distribution, and analyze the relationship between the electric field (the trapping potential) and the parameters of charged wires layout. Also, the study shows that there is a point of zero electric field at the position (0, y_0), this spatial electric field distribution looks like a hollow electrostatic tube with a zero central electric field, which can be used to guide cold polar molecules in the weak-field-seeking state along the z-direction, and obtain a higher guiding efficiency. Moreover, the surface guiding scheme can also be used to form various molecule-optical elements, such as molecular funnel, molecular beam-splitter, molecular interferometer, even to develop some integrated molecule chips.

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