PHYSICAL REVIEW LETTERS

Electrostatic Surface Guiding for Cold Polar Molecules: Experimental Demonstration

Yong Xia, Yaling Yin, Haibo Chen, Lianzhong Deng, and Jianping Yin*

State Key Laboratory of Precision Spectroscopy, Department of physics, East China Normal University, Shanghai 200062, P.R. China

We demonstrate an electrostatic surface guiding for cold polar molecules over a long distance of 44.5 cm, 0.85 mm above a dielectric substrate, and measure the transverse distribution of the guided supersonic D_2O/CH_3Br beam and its longitudinal velocity one. Also, we study the dependence of the relative guiding efficiency and the transverse temperature of the guided molecular beam on the guiding voltage, and show that the absolute guiding efficiencies from the Monte Carlo simulation and theoretical calculation multiplied by 3 are about equal to the measured relative one.
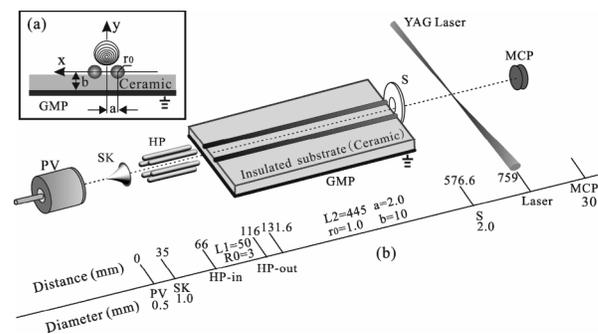
Cold molecules offer new opportunities for cold molecular spectroscopy and precision measurements [1], molecular collisions and cold chemistry [2,3], quantum computing and its information processing [4,5], and so on. Especially, cold polar molecules have attracted increasing interest in the recent years. Using the interaction of their electric dipole moments (EDM) with an inhomogeneous electrostatic field, polar molecules can be decelerated [6], trapped [7], and manipulated [8–13]. In 2000, Loesch *et al.* demonstrated the Keppler-type electrostatic guiding of cold polar molecules (NaCl, NaBr and NaI) in the strong-field-seeking (SFS) states [8]. Recently, Rempe's group realized the guiding of several polar molecules (H_2CO and ND_3, etc.) in the weak-field-seeking (WFS) states or in the SFS ones from an effusive molecular beam by using a standard quadrupole electrostatic field [9,10]. Their schemes can not only be used to guide and manipulate cold molecules in the SFS or WFS states, but also to generate a continuous wave (CW) cold molecular beam by the low-pass energy filter based on the molecular bend guiding. However, none of the guiding schemes mentioned above can be used to realize an electrostatic surface guiding, splitting, and interfering of cold polar molecules on a molecular chip. So it would be interesting and worthwhile to propose, demonstrate and study some novel electrostatic surface guiding for cold polar molecules on a chip.

In 2005, a novel scheme [13] to guide cold polar molecules using a hollow electrostatic tube was proposed. In this Letter, we demonstrate the first molecular surface guiding scheme mentioned above and report some new experimental results on the electrostatic guiding of a supersonic D_2O or CH_3Br beam in the WFS states, and study the dependences of the relative guiding efficiency and the transverse temperature of the guided molecular beam on the guiding voltage. Finally, we briefly discuss some potential applications of our guiding scheme in molecule optics.

The experimental setup to guide cold polar molecules on the surface of an insulated ceramic substrate is shown in Fig. 1, which consists of two differentially pumped vacuum chambers, including a compact supersonic molecular beam, a molecular guiding and detecting system. The operating pressure in the source chamber and the guiding one are typically $\sim 2.0 \times 10^{-3}$ Pa and $\sim 3.0 \times 10^{-6}$ Pa, respectively. A pulsed supersonic molecular beam is formed by adiabatically expanding a gaseous mixture, 1.2% D_2O (or 5.0% CH_3Br) evaporated at room temperature with argon carrier gas through a solenoid valve (General Valve, Series 9) into vacuum, and the stagnation pressure is 2.0 atm. Locations of each element with respect to the nozzle of the valve and their sizes are showed in Fig. 1(b). The generated molecular beam passes through a skimmer with a diameter of 1.0 mm into the guiding chamber, and flies into a 50-mm-long hexapole, which is made of six stainless-steel rods with 3.0 mm diameter placed equidistantly on a circle with 4.5 mm radius. Such hexapole rods, as a positive electrostatic lens, are used to select the WFS molecules and focus them into a 2D hollow electrostatic field. The output molecular beam from a

FIG. 1. (a) Cross-sectional view of two parallel charged wires and a grounded metal plate. The two wires are embedded in an insulated ceramic substrate by a depth of about $r_0/2 = 0.5$ mm, and the distance between the guiding center of cold molecules and the surface of the ceramic substrate is 0.85 mm. (b) The experimental setup and the locations of each element in front of the nozzle and their sizes. PV, SK, HP, GMP, S stand for pulse valve, skimmer, hexapole, grounded mental plate, and sampling hole.

043003-1

sampling small hole with a diameter of 2.0 mm is ionized by the frequency-quadrupled pulsed light of an Nd:YAG laser (Surelite I-10, 266 nm, 10 Hz) with a single-pulse energy of 10.5 mJ, and then the molecular ions are extracted and accelerated into a homemade time-of-flight (TOF) mass spectrometer with Wiley-McLaren type; the ions are then measured by dual micro-channel plates (MCP) detector, and the signals are collected and averaged over 300 shots on an oscilloscope (HP 54616C, 500 MHz), whose output is transferred to the person's computer for signal storage and processing.

The cross-sectional diagram of the guide apparatus is shown in Fig. 1(a), the length of the guiding electrodes and their radius are $L = 445.0$ mm and $r_0 = 1.0$ mm respectively, and the distance between the grounded metal plate and the center of the guiding electrodes is $b = 10.0$ mm. The central spacing between the two charged electrodes is $2a = 4$ mm, the two electrodes are embedded in an insulated ceramic substrate by a depth of about $r_0/2 = 0.5$ mm, the relative dielectric constant of the used ceramic substrate is $\epsilon_r = 6.2$, and its dielectric strength is greater than 60 kV/cm. In this case, the guiding center of cold molecules is above the surface of the ceramic substrate by 0.85 mm. We use the finite element software to calculate the spatial electrostatic field distribution of our charged-

wire layout, and find that there is a two-dimensional (2D) hollow electrostatic field distribution with a central minimum above the center between the two wires [see Fig. 1(a)], which can be used to realize an electrostatic surface guiding of cold polar molecules. The interaction potential of the guided molecules with the electrostatic field depends on the molecular internal quantum state, while the molecular transverse motion will be confined by the guiding Stark potential. When guiding voltage is high enough, some hot molecules with mean transverse kinetic energy higher than the maximum transverse potential depth cannot be guided in our hollow electrostatic pipe, while most of cold molecules with lower transverse kinetic energies can be efficiently guided. It is clear that the guiding effect of cold molecules mainly happens in the transverse direction. In the experiment, consequently, we mainly measure and study the transverse distribution of the guided molecular beam under the different guiding voltages.

When cold molecules are regarded as classical particles in the course of the guiding, the velocity distributions of the molecules before and after the guide are written as $f(v_x, v_y, v_z)$ and $f'(v_x, v_y, v_z)$, respectively. Since the motion of the guided molecules in the velocity region $S(x, y)$ satisfies the energy conservation law, the absolute guiding efficiency can be defined and expressed as

$$\eta_{\text{eff}} \equiv J_{\text{out}}/J_{\text{in}} = \frac{\int_{A'(x,y)} f'_p(x, y)dxdy \int_{S'(v_x,v_y),v_z>0} f'(v_x, v_y, v_z)v_z dv_x dv_y dv_z}{\int_{A(x,y)} f_p(x, y)dxdy \int_{S(v_x,v_y),v_z>0} f(v_x, v_y, v_z)v_z dv_x dv_y dv_z}, \tag{1}$$

where $A(x, y)[A'(x, y)]$ is the spatial integrated region of the guided molecules at the inlet [outlet] of the electrostatic tube, J_{in} and J_{out} are the input and output fluxes of the guided molecular- beam, and $f_p(x, y)$ and $f'_p(x, y)$ are the 2D position distributions of the molecular beam at the inlet and outlet of the electrostatic tube, respectively.

In the experiment, the open width of the pulse valve is 400 μs, the mean velocity of the D_2O beam is around 550 m/s with a velocity spread (FWHM) of about 28% at a translational temperature of 16.3 K, and the transverse temperature is about 61.3 mK, which was measured after the skimmer. In the supersonic expansion, the molecular beam is rotationally and vibrationally cooled, and after the hexapole electrostatic field, more than 97% molecules in our guided molecular beam are populated in the WFS states of $J \leq 2$ [14]. The experimental results of the transverse distribution of the guided D_2O molecules and its dependence on the guiding voltage are shown in Fig. 2. We can find from Fig. 2 that the higher the guiding voltage is, the higher the relative ion signal intensity is, and all transverse distributions of the guided D_2O beam are Gaussian ones. It is clear that the integrated area of each transverse distribution is proportional to the flux J (or the number N) of the guided D_2O molecules, and this guiding flux depends on the transverse Stark trapping potential for

D_2O molecules, which will be determined by the applied guiding voltage on the two electrodes. Also, we measure the longitudinal velocity distribution of the guided D_2O
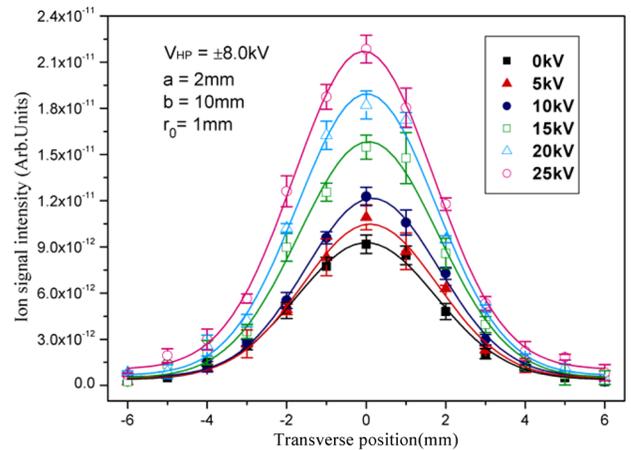

FIG. 2 (color online). Relative ion signal intensity of the guided D_2O molecules versus the transverse position for $V_{\text{guide}} = 0, 5, 10, 15, 20$ and 25 kV when $a = 2$ mm, $b = 10$ mm, $r_0 = 1$ mm, and $V_{\text{HP}} = \pm 8.0$ kV. Various symbols are the experimental data, including the corresponding error bars, and the solid lines are the fitted curves by Gaussian profile.

molecular beam and its dependence on V_{guide}, and find that the guided molecular number is slightly increased with the increase of the guiding voltage, and the longitudinal most probable velocity of the guided molecular beam and its translational temperature are nearly unchanged.

We study the dependence of the relative guiding efficiency of cold molecules on the guiding voltage, and the measured, calculated, and Monte Carlo simulated results are shown in Fig. 3, here the integrated area under each transverse profile as shown in Fig. 2 is proportional to the number N of the guiding molecules, and the relative guiding efficiency is defined as the ratio of the area subtracting the integrated area without guiding voltage from one at each V_{guide} to the integrated area at $V_{guide} = 25.0$ kV. It is clear from Fig. 3 that the higher the guiding voltage is, the higher the relative guiding efficiency is, and our experimental results are in good agreement with the both calculated and simulated ones when they are multiplied by 3. The absolute guiding efficiencies from the theoretical calculation and simulation are ~33%, which multiplied by 3 is about equal to our measured relative efficiency as $V_{guide} = 25$ kV. In particular, when the guiding voltage is lower, some hotter molecules in the molecular beam will be stuck on the surface of the ceramic substrate, and then lost from our guided molecular beam. Also, we observed the transverse velocity distribution of the guided D_2O molecular beam, and studied the dependence of the transverse temperature on the guiding voltage, and the experimental results are shown in Fig. 4. The transverse temperature
of the guided molecular beam is increased with the increase of the guiding voltage, such as the transverse temperature is increased from about 5.7 mK to 13.5 mK
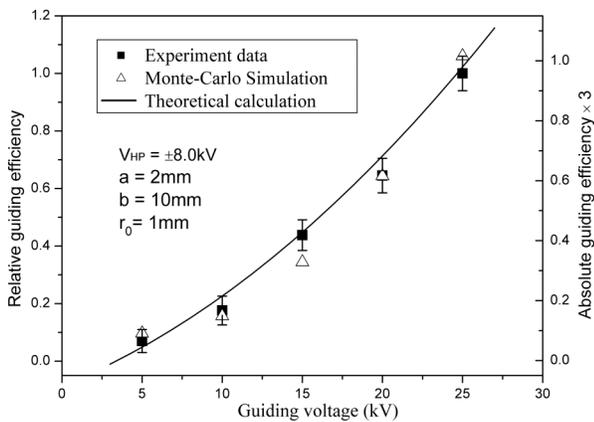
when the guiding voltage is increased from 5 kV to 25 kV. This is because the higher the guiding voltage, the deeper the transverse well depth of our guiding system, and then the higher the guiding efficiency, the higher the transverse temperature of the guided molecular beam. In particular, when $V_{guide} = 25$ kV, the transverse temperature of the guided molecular beam is ~13.5 mK, which is slightly greater than the maximum transverse trapping potential (11.5 mK) for cold D_2O molecules in the $|J = 1, \tau = 1, M = 1\rangle$ state where the definitions of quantum numbers (J, τ, M) can be found in Ref. [11]), while the transverse potentials for the D_2O molecules in all other WFS states are lower than 11.5 mK.

In addition, we study the dependence of the relative guiding efficiency of D_2O and CH_3Br molecules on the guiding voltage when the hexapole voltage is switched off, and the experimental and simulated results are shown in Fig. 5. In the experiment, a pulsed supersonic CH_3Br beam was produced by expanding a 5% CH_3Br in Ar mixture into vacuum, the most probable velocity of the CH_3Br beam is about 550 m/s with a velocity spread (FWHM) of about 20%, corresponding to a translational temperature of ~6 K. From Fig. 5, we can find that the guided molecular signals are enhanced with the increasing of the guiding voltage, and the maximum (simulated) absolute guiding efficiency can reach about 40% and 20% as $V_{guide} = 25$ kV and $V_{HP} = 0$ kV for CH_3Br and D_2O beam, respectively. Under the same guiding voltage, the relative guiding efficiency of the CH_3Br molecules is far higher than that of the D_2O molecules, because the Stark guiding potential for CH_3Br molecules is far higher than that for D_2O molecules under the same experimental conditions. In final, we also study the influence of the hexapole voltage on the guiding efficiency under the same conditions, and find that the relative guiding efficiency of cold D_2O molecules when

FIG. 3. Dependence of the relative guiding efficiency of cold molecules on the guiding voltage for $a = 2$ mm, $b = 10$ mm, $r_0 = 1$ mm, and $V_{HP} = \pm 8.0$ kV. The measured experimental data (solid squares) with an error bar is the relative guiding efficiency (on the left side of figure), and the simulated data (hollow triangles) and theoretical calculation (solid line) are the absolute efficiency (on the right side of figure), which was multiplied by 3.
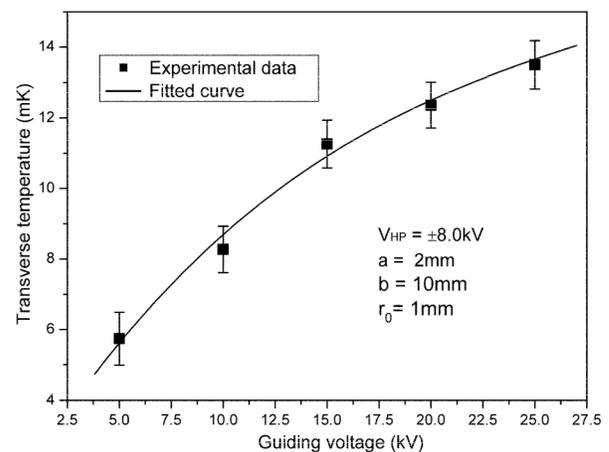
FIG. 4. Dependence of the transverse temperature of the guided molecular beam on the guiding voltage for $a = 2$ mm, $b = 10$ mm, $r_0 = 1$ mm, and $V_{HP} = \pm 8.0$ kV. The black squares with an error bar are the experimental data, and the solid line is fitted curve.
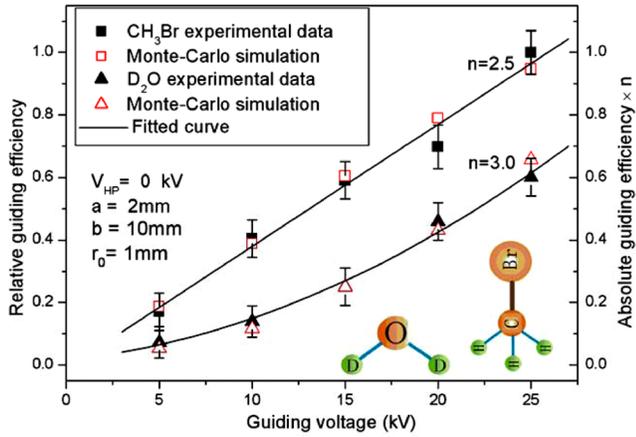
FIG. 5 (color online). Dependence of the relative guiding efficiency of cold molecules on the guiding voltage for D_2O and CH_3Br molecular beam when $V_{HP} = 0$ kV, $a = 2$ mm, $b = 10$ mm, and $r_0 = 1$ mm. The measured experimental data (solid squares or triangles) with an error bar is the relative guiding efficiency (on the left side of figure), and the simulated data (hollow squares or triangles) is the absolute efficiency (on the right side of figure), which was multiplied by 3 for D_2O and by 2.5 for CH_3Br. The solid lines are fitted curves.

$V_{HP} = \pm 8$ kV is higher than that as $V_{HP} = 0$ kV by about 1.6 times. This shows that the focusing or coupling effect of the charged hexapole for incident molecular beam is very important; it can be used to efficiently enhance the guiding efficiency of cold polar molecules in the 2D hollow electrostatic tube. Also, we can find from Figs. 5 that our experimental data are consistent with our simulated results.

In conclusion, we have demonstrated a novel electrostatic surface guiding scheme for cold D_2O and CH_3Br molecules on the surface of the ceramic substrate, and obtained some new experimental results consistent with theoretical and simulated ones. Our study shows that (1) the relative guiding efficiency of cold molecules is increased with the increasing of the guiding voltage, and the calculated and simulated absolute guiding efficiencies are $\sim 33\%$, which multiplied by 3 is about equal to our measured relative efficiency as $V_{guide} = 25$ kV. (2) The corresponding transverse temperature of the guided D_2O beam is increased by ~ 2.4 times, while the longitudinal most probable velocity and its temperature are nearly unchanged. (3) The relative guiding efficiency of CH_3Br molecules is higher than that of D_2O molecules by ~ 2.0

times under the same guiding voltage, and the (simulated) absolute guiding efficiency of CH_3Br molecules can reach to be 40% as $V_{guide} = 25$ kV. Moreover, the relative guiding efficiency of cold D_2O molecules when $V_{HP} = \pm 8$ kV is higher than that as $V_{HP} = 0$ kV by ~ 1.6 times under the same guiding conditions.

Our surface guiding scheme can be miniaturized and integrated on the surface of a chip, and obtain a higher guiding efficiency, so it can be used to form various molecule-optical elements, such as molecular funnel using a ladder-shaped double-wire guiding scheme, Y-shaped molecular beam splitter [15] with a Y-shaped double-wire guiding scheme, and molecule interferometer using two Y-shaped beam splitters and so on, even to generate a CW cold molecular beam on a molecular chip by using an electrostatic bent guide. Therefore, our guiding scheme has some new and important applications in molecule optics, quantum computing, and quantum information processing, even to open a new field for studying integrated molecule optics and its molecular chip.

*Corresponding author: jpyin@phy.ecnu.edu.cn

[1] J. J. Hudson *et al.*, Phys. Rev. Lett. **89**, 023003 (2002).
[2] J. J. Gilijamse *et al.*, Science **313**, 1617 (2006).
[3] E. R. Hudson *et al.*, Phys. Rev. A **73**, 063404 (2006).
[4] D. DeMille, Phys. Rev. Lett. **88**, 067901 (2002).
[5] A. Andre *et al.*, Nature Phys. **2**, 636 (2006).
[6] H. L. Bethlem *et al.*, Phys. Rev. Lett. **83**, 1558 (1999).
[7] H. L. Baethlem *et al.*, Nature (London) **406**, 491 (2000).
[8] H. J. Loesch and B. Scheel, Phys. Rev. Lett. **85**, 2709 (2000).
[9] S. A. Rangwala *et al.*, Phys. Rev. A **67**, 043406 (2003).
[10] T. Junglen *et al.*, Phys. Rev. Lett. **92**, 223001 (2004).
[11] T. Rieger *et al.*, Phys. Rev. A **73**, 061402 (2006).
[12] D. Hain, Ph.D. thesis, University of Utah, 2000.
[13] Y. Xia, L. Z. Deng, and J. P. Yin, Appl. Phys. B **81**, 459 (2005).
[14] W. Gordy and R. L. Cook, *Microwave Molecular Spectra* (Wiley Publications, New York, 1984), 3rd ed..
[15] L. Deng and J. Yin, Opt. Lett. **32**, 1695 (2007).