Trapping of cold molecules
Optimizing the Stark decelerator beamline using evolutionary strategies

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Berlin

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Germany – Ecuador 3:0
Poland – Costa-Rica 2:1

1. Germany 9 points
2. Ecuador 6 points
3. Poland 3 points
4. Costa Rica 0 points
Applications of cold molecules

- Getting complete control over both the internal and external degrees of freedom of molecules:
  - Beams of molecules in a single (or a small subset of) quantum states
  - Spatially oriented molecules
  - Beams/packets of molecules with a computer controlled velocity distribution

- Slow molecular beams for metrology; sensitive symmetry tests:
  - Weak interactions in chiral molecules
  - Time-reversal violating electric dipole moment of the electron (EDM)
  - Time-variation of fundamental constants (i.e. $\frac{da}{dt}$)

- Novel molecular beam collision, reaction, and interferometry experiments:
  - Conformational interchange and dynamics (folding)
  - Collisions at variable, well-defined energies
  - Scattering resonances
  - Quantum-controlled chemistry

- Ultra-low temperature phenomena:
  - Anisotropic dipole-dipole interaction:
    - repulsive: $\uparrow\uparrow$
    - attractive: $\rightarrow\rightarrow$
  - Molecular BEC
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Interaction of molecular charge distribution with external electric field:

\[ U_{pot} = W_{\text{Stark}} \]

\[ W_{\text{Stark}} = -\vec{\mu} \cdot \vec{E} \]

\[ F_{\text{Stark}} = -\frac{\partial W_{\text{Stark}}}{\partial z} \]
Interaction of molecular charge distribution with external electric field:
Deceleration principle

interaction of molecular charge distribution with external electric field:

\[ \text{HV} \cdot \text{HV} \]

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<table>
<thead>
<tr>
<th>M</th>
<th>3/2</th>
<th>1/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>energy (cm(^{-1}))</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>electric field strength (kV/cm)</td>
<td>0</td>
<td>50</td>
</tr>
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</table>

high-field-seeking

low-field-seeking

Jochen Küpper (Fritz-Haber-Institut der MPG)

Optimizing the Stark decelerator beamline

Columbus, OH — 20. June 2006
Deceleration principle

**Introduction**

Stark deceleration

**Deceleration principle**

Interaction of molecular charge distribution with external electric field:

$$U_{pot} = W_{Stark}$$

$$W_{Stark} = -\vec{\mu} \cdot \vec{E}$$

$$F_{Stark} = -\frac{\partial W_{Stark}}{\partial z}$$

**Diagram**

- High-field-seeking
- Low-field-seeking

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<td>energy (cm$^{-1}$)</td>
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Time 1

- HV
- HV
- -HV
- -HV

Time 2

- HV
- HV
- -HV
- -HV

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Optimizing the Stark decelerator beamline

Columbus, OH — 20. June 2006
Experimental setup

Stark decelerator

Pulsed valve
Hexapole
Skimmer

Photodissociation laser (193 nm)

1.31 m

Detection laser

LIF zone

Trap

PMT
Experimental setup

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Columbus, OH — 20. June 2006
Experimental setup

Phase-space evolution
### Stark deceleration

- OH radicals in a *single quantum state* are trapped in the traveling potential well of the decelerator.
- Translational temperatures $\sim 100$ mK.
- Molecules can be decelerated to any computer-controlled velocity.
- $10^6$ OH radicals per packet.
- Density of $10^7–10^8$ cm$^{-1}$.

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Experimental results

Deceleration and Trapping

Trap loading and trapping

Pulsed valve
Hexapole
Skimmer
Stark decelerator (108 stages)
LIF zone
Photodissociation laser (193 nm)
Detection laser

**Graph:**
- **LIF signal (a.u.)**
- **time (ms):** 6.0, 7.0, 8.0, 9.0

**(i)**

**Table:**

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<thead>
<tr>
<th>Time (ms)</th>
<th>LIF Signal (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.0</td>
<td>0.2</td>
</tr>
<tr>
<td>7.0</td>
<td>0.4</td>
</tr>
<tr>
<td>8.0</td>
<td>0.6</td>
</tr>
<tr>
<td>9.0</td>
<td>0.8</td>
</tr>
</tbody>
</table>

**Equation:**

\[ \tau = 1.6 \text{ s} \]

Experimental results
Deceleration and Trapping

Optimizing the Stark decelerator beamline

Experimental results
Deceleration and Trapping

Trap loading and trapping

(i)

(ii)

(iii)

LIF signal (a.u.)

time (ms)

6.0 7.0 8.0 9.0

loading

trapping

7 kV 15 kV -15 kV

-15 kV 15 kV -15 kV

Position (mm)

Energy (cm⁻¹)

0 0.2 0.4 0.6

0 0.2 0.4 0.6

-12 0 12

-12 0 12

Experimental results
Deceleration and Trapping

**Trap loading and trapping**

A

(i)

(ii)

(iii)

LIF signal (a.u.)

6.0 7.0 8.0 9.0
time (ms)

0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8
time (s)

\( \tau = 1.6 \text{s} \)

Experimental results

Direct lifetime measurements

The vibrational lifetime of $\text{OH} \: X^2\Pi_{3/2}, \nu = 1, J = 3/2$

$\tau_{\text{vib}} = 59 \text{ ms}$

$\tau = 1.3 \pm 0.1 \text{s}$

$\tau = 56.4 \pm 1.9 \text{ ms}$

$\text{Meerakker et al, Phys. Rev. Lett. 95, 013003 (2005)}$
Direct lifetime measurements
The vibrational lifetime of OH $X^2\Pi_{3/2}, v = 1, J = 3/2$

The vibrational lifetime of OH $X^2\Pi_{3/2}, v = 1, J = 3/2$ was measured using a pulsed valve, hexapole skimmer, Stark decelerator, LIF zone, and PMT. The photodissociation laser (193 nm) and detection laser (346 nm) were used to excite and detect OH molecules.

The storage time versus LIF signal for OH $X^2\Pi_{3/2}, J = 3/2, v = 0$ and OH $X^2\Pi_{3/2}, J = 3/2, v = 1$ are shown in the graph. The vibrational lifetime $\tau_{vib}$ is calculated as follows:

$\tau_{vib} = 59 \text{ ms}$ for OH $X^2\Pi_{3/2}, J = 3/2, v = 0$

$\tau_{vib} = 1.3 \pm 0.1 \text{ s}$

$\tau_{vib} = 56.4 \pm 1.9 \text{ ms}$ for OH $X^2\Pi_{3/2}, J = 3/2, v = 1$

Optimizing the Stark decelerator beamline

Experimental results
Automated optimization

Parameter encoding
Parameter reduction

- Encode deceleration in polynomial:
  Decelerator 1 \((i = 1–102)\):

\[ t_i = t_{i,0} + \sum_{j=0}^{o_1} p_{j+1} \cdot (i - 1)^j \]

Decelerator 2 \((i = 103–106)\):

\[ t_i = t_{i,0} + \sum_{j=0}^{o_2} p_{j+o_1+2} \cdot (i - 103)^j \]

- Directly use \(\Delta t\)'s for last timings 
  \((i = 107–111)\):

\[ \Delta t_i = t_i - t_{i-1} = p_{i+o_1+104} \]

Full parameter vector

\[ \vec{P} = (p_1, p_2, \ldots, p_{o_1+101})^T \in (\mathbb{R}^+)^{o_1+102} \]

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Experimental results

Automated optimization

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Parameter reduction

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**Full parameter vector**

\[ \vec{P} = (p_1, p_2, \ldots p_{o_1+o_2+7})^T \in (\mathbb{R}^+)^{o_1+o_2+7} \]

Evolutionary Algorithms

- Initial population
- Evaluation
- Parents
- Replacement
- Evaluation
- Selection and crossover
- Mutation
- Offspring
- Final population
- Stop?

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Columbus, OH — 20. June 2006
Implementation of experimental feedback-control system

- Completely computer-controlled experiment:
  - Homebuilt burst-units to control high-voltage switches
    4 channels per unit, 10 ns resolution, FPGA-based 6U-cPCI cards
  - User-friendly homebuilt control and data-acquisition software KouDA
    C++, Qt, VxWorks, Linux → http://kouda.cold-molecules.info

- Evolutionary-computation framework:
  - Evolving Objects → http://eodev.sourceforge.net

- eoEsStdev algorithm: Evolutionary Strategy with
  - individual mutation widths for all parameters
  - optimization of mutation widths as meta-parameters
  - no correlation of parameters utilized

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Experimental results

Automated optimization

1.31 m
pulsed valve
hexapole
skimmer
Stark decelerator
LIF zone
PMT
photodissociation
laser (193 nm)
detection laser
(282 nm)
trap
hexapole Stark decelerator 1 trap Stark decelerator 2

LIF intensity
(fitness)

10 Hz

trial timesequence

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Implementation of experimental feedback-control system

Experimental results

Automated optimization

1.31 m
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PMT
photodissociation laser (193 nm)
detection laser (282 nm)
trap
hexapole
Stark decelerator 1
Stark decelerator 2

LIF intensity
(fitness)

10 Hz

50 generations
1–2 h

trial timesequence

10 Hz

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Optimizing the Stark decelerator beamline

Columbus, OH — 20. June 2006

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Optimization results

Optimization results

Optimization results

Conclusions

- Time-varying electric fields can be used to decelerate and trap neutral polar molecules.

- OH radicals have been trapped at a density of $10^7–10^8 \text{ cm}^{-3}$ and a temperature of 50–500 mK.

- The switching times of the Stark decelerator beamline have been optimized using evolutionary strategies.

- The number of trapped OH radicals has been increased by 40%.


- Advanced optimization objectives:
  - Minimize temperature of trapped packet
  - Optimize number of trapped molecules and temperature simultaneously
  - Optimize intensity of decelerated packets using cw detection techniques.
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