Fundamental physics with diatomic molecules:

from particle physics to quantum computation….!

- electron electric dipole moment search ($\not{C}\not{P}$, "new" physics)
- sources of ultracold molecules for wide range of applications:
  - --large-scale quantum computation
  - --time variation of fundamental "constants"
  - --etc.
- parity violation: Z^0 couplings & nuclear anapole moments

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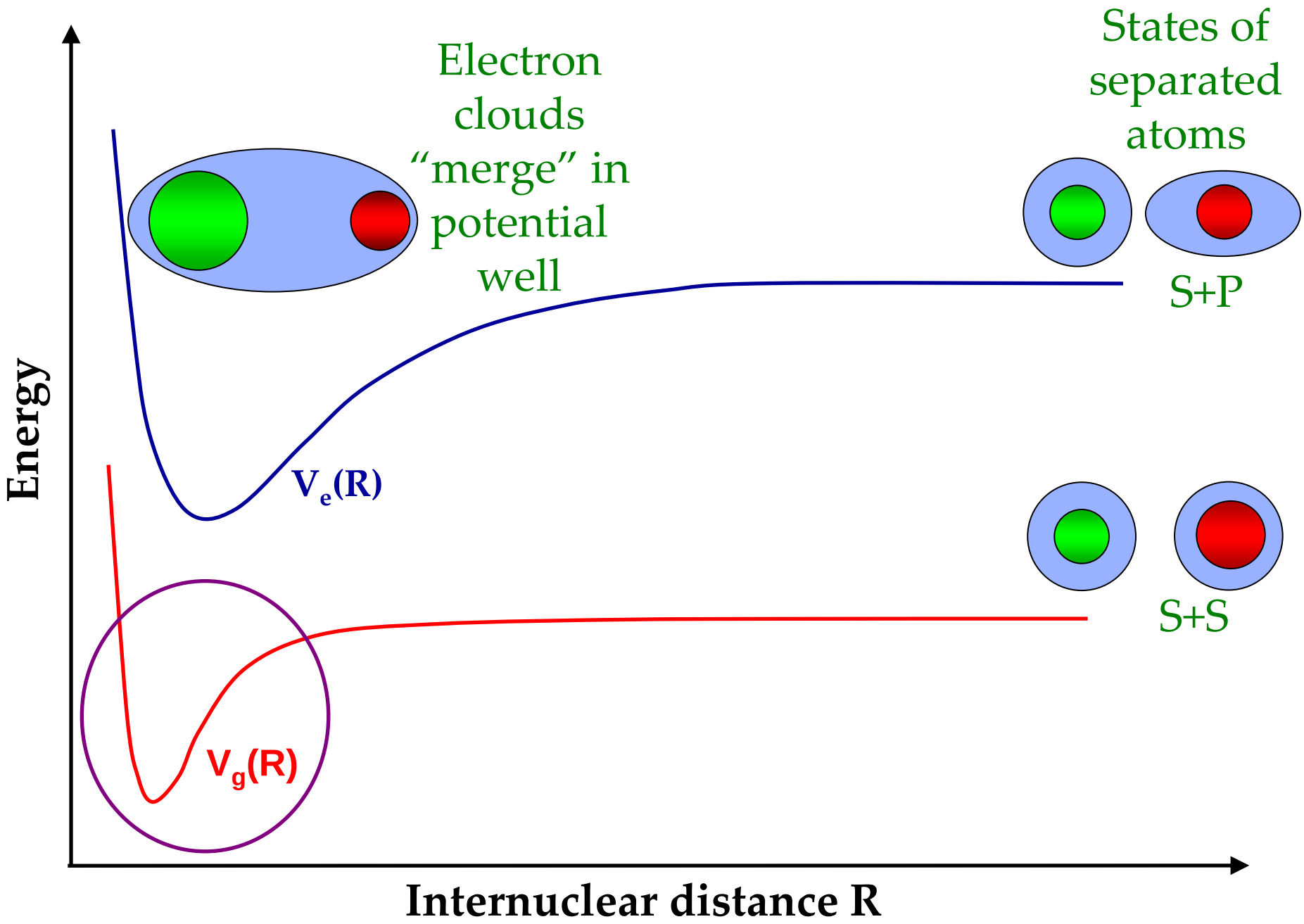
Structure of molecules 0:

"A diatomic molecule has one atom too many."
--Art Schawlow
(and most atomic physicists)

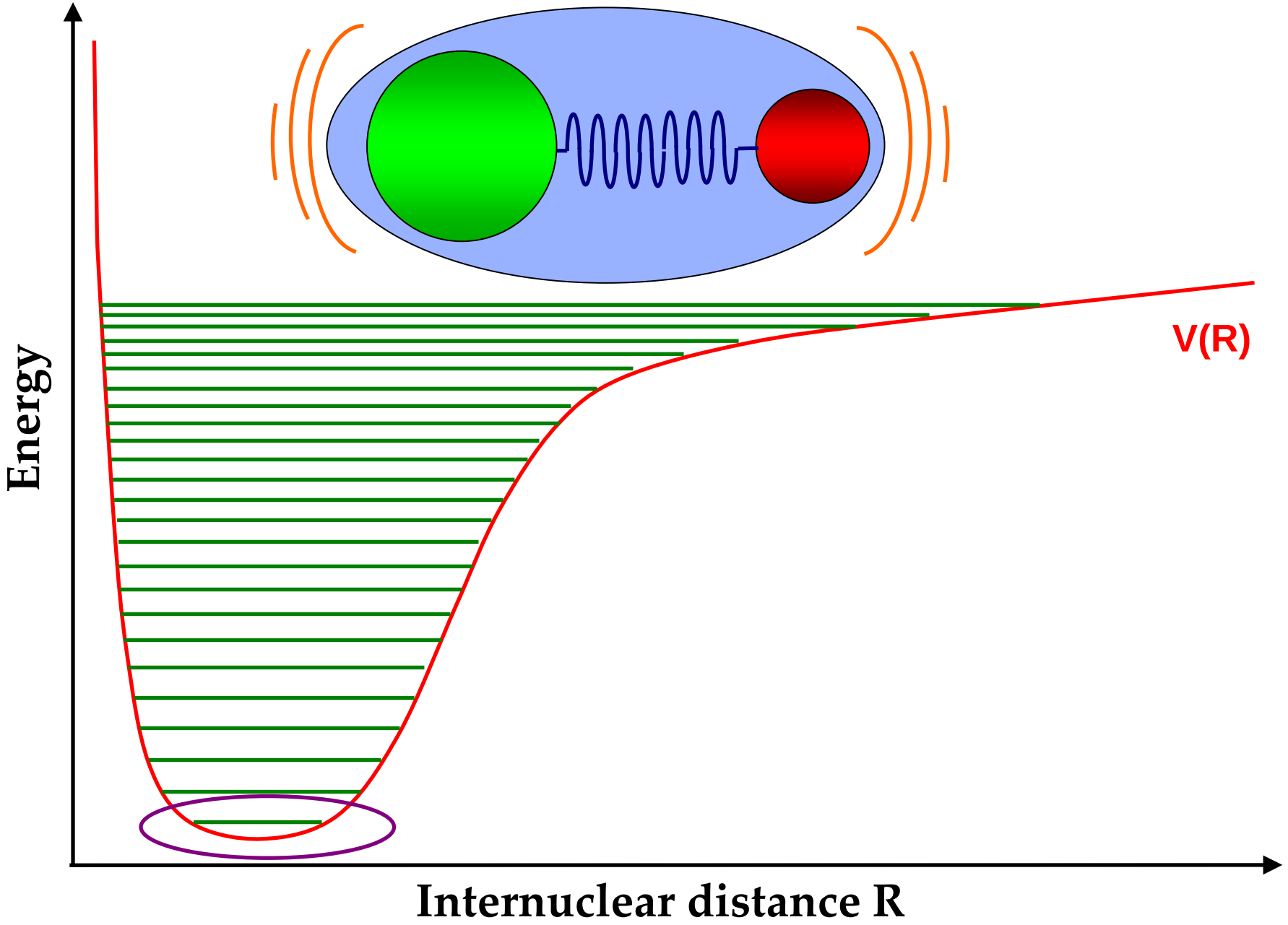
....or maybe not?

"new" internal degrees of freedom in molecules useable as a resource*...?*

Structure of molecules I: electronic states



Structure of molecules II: vibration



Structure of molecules III: rotation

Moment of intertia

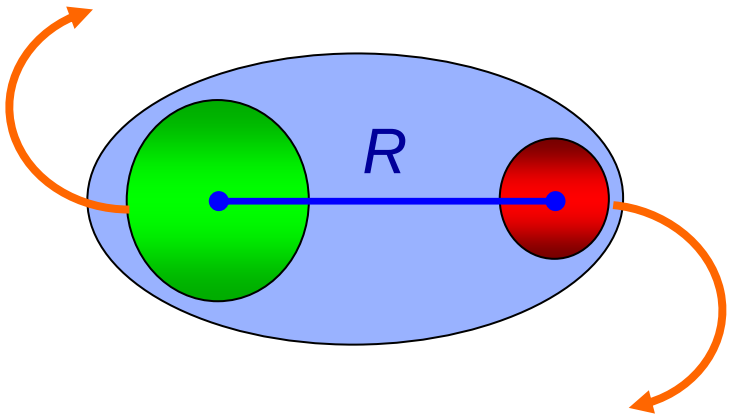
$I = MR^2$;

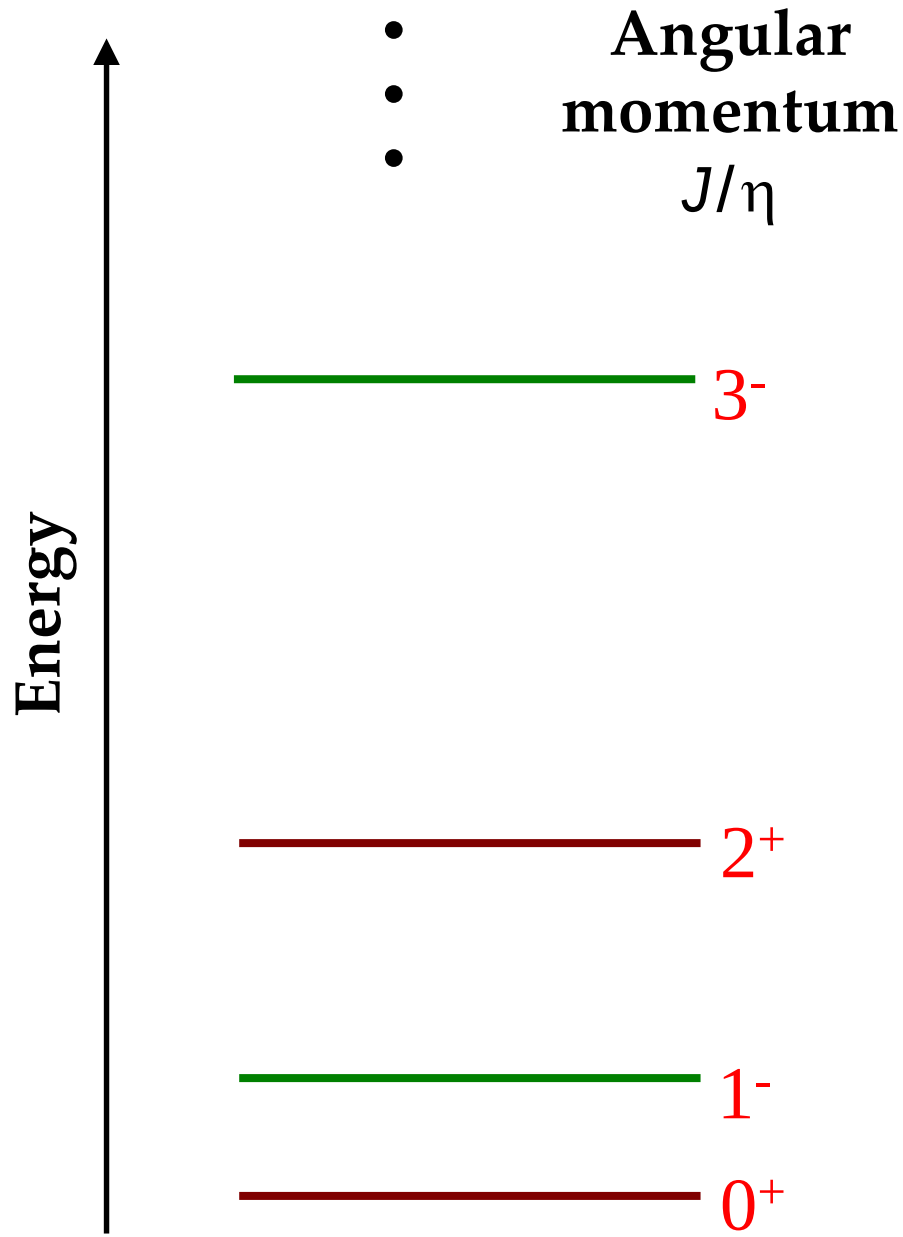
Angular momentum

$J = n\eta$;

Energy of rotation

$E = J^2/2I$





Molecular electric dipoles

Wavefunctions of polar molecules

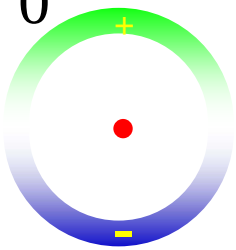
No E-field: no dipole!

With E-field: induced dipole

polarized molecules act like permanent dipoles

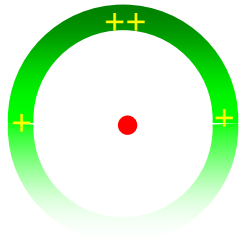
$J = 1, m_J = 0$

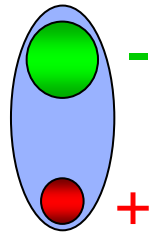
"=" $|p\rangle$



z, E

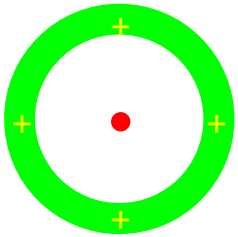
$|\downarrow\rangle \propto |s\rangle + |p\rangle$



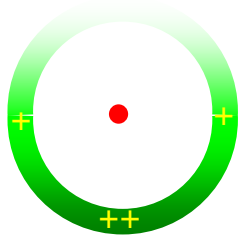


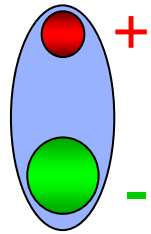
$J = 0$

"=" $|s\rangle$



$|\uparrow\rangle \propto |s\rangle - |p\rangle$



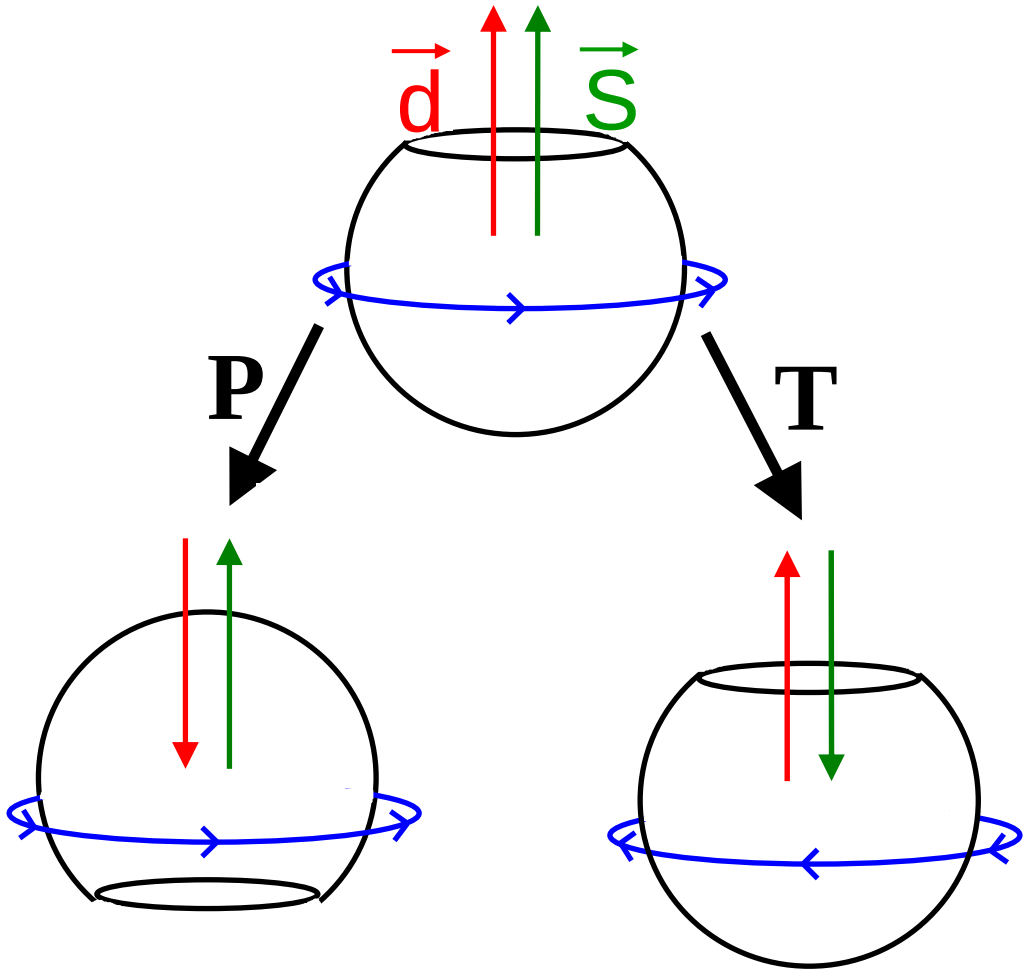


Small splitting (~10^{-4} eV) between states of opposite parity (rotation) leads to *large polarizability* (vs. atoms, ~ few eV)

A permanent EDM Violates T and P

Purcell
Ramsey
Landau

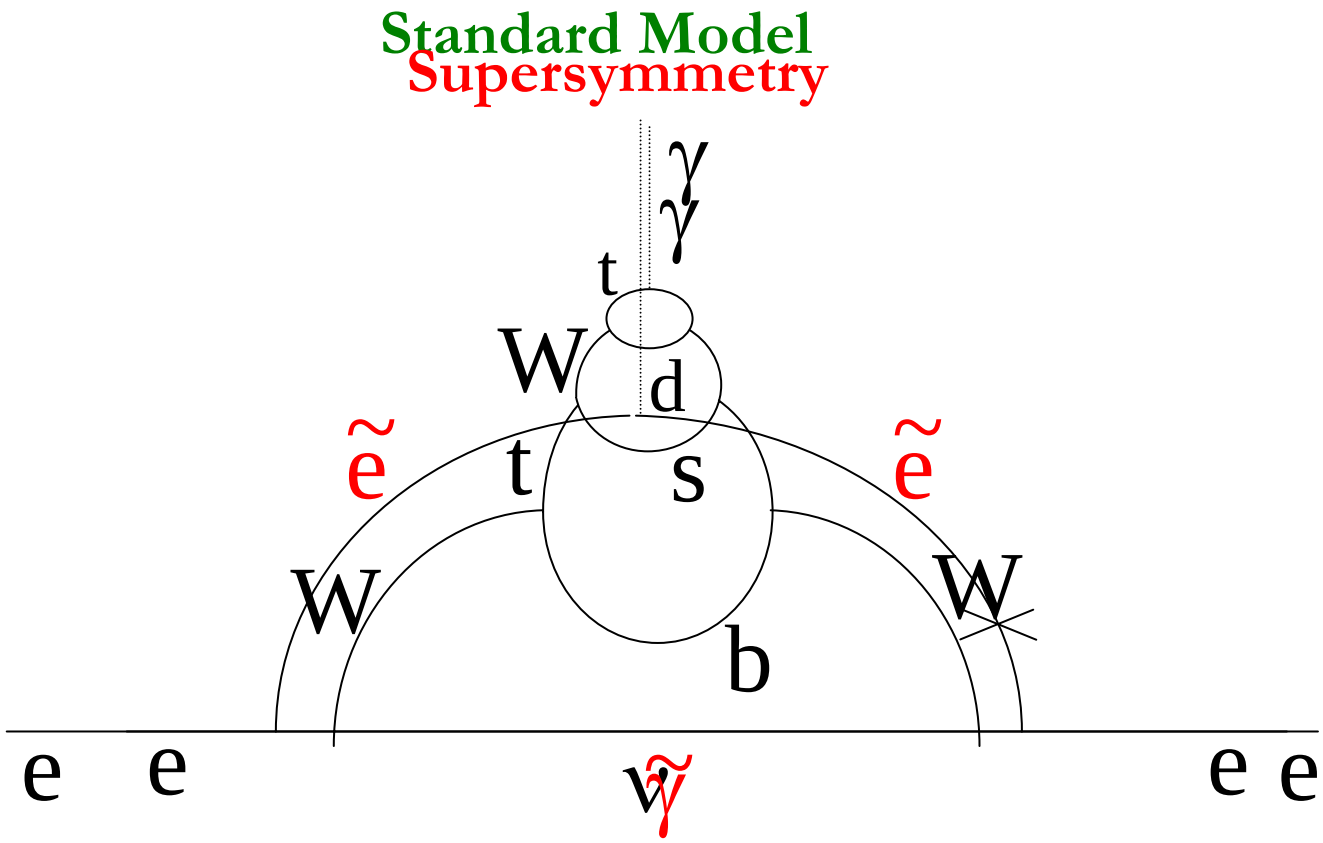
$$H_{Magnetic\ dipole} = -\vec{\mu}\cdot\vec{B} = -\mu\vec{\sigma}\cdot\vec{B} \qquad H_{Electric\ dipole} = -\vec{d}\cdot\vec{E} = -d\vec{\sigma}\cdot\vec{E}$$



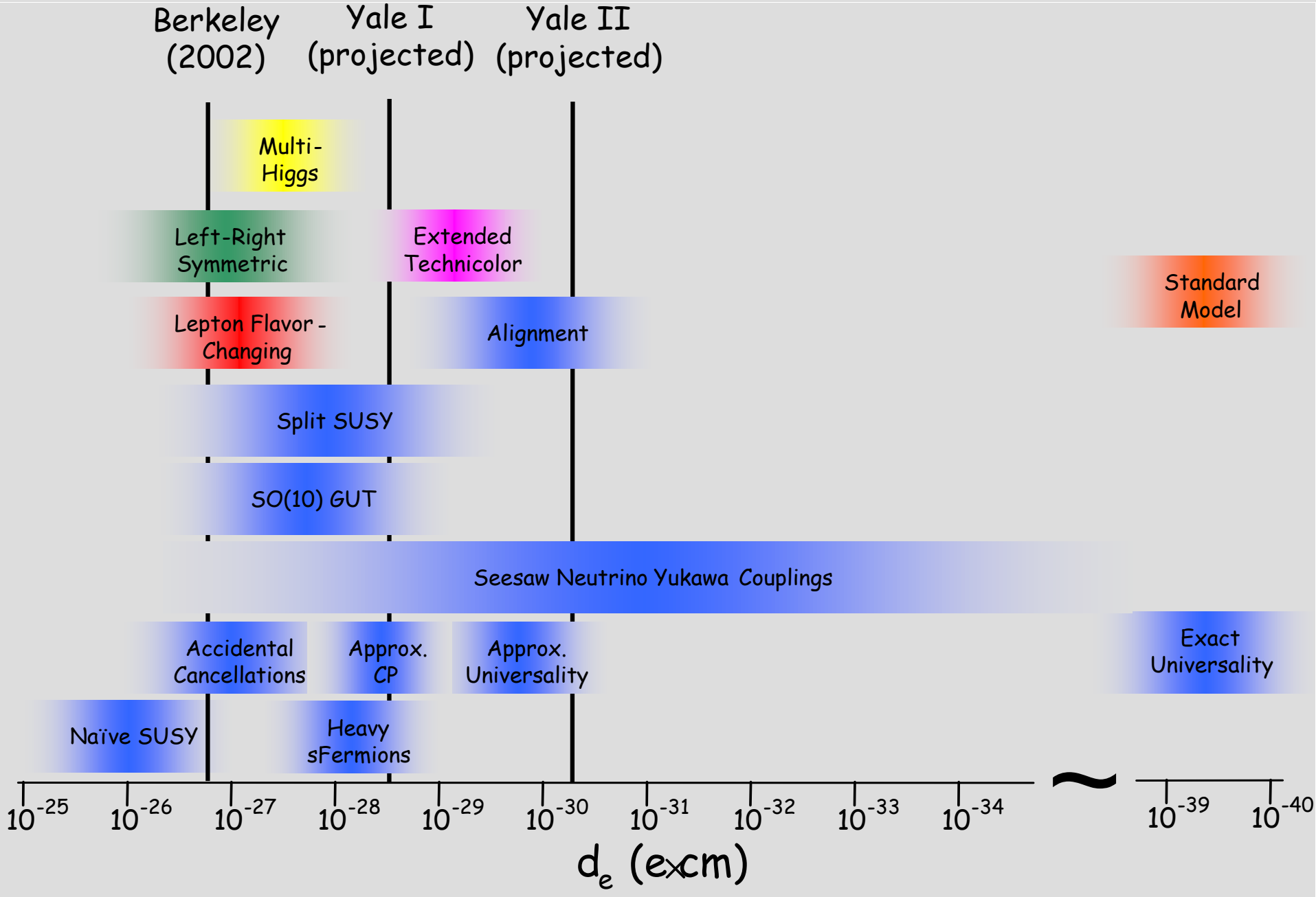
CPT theorem $\Rightarrow$ T-violation = CP-violation

Q. How does an electron EDM arise?

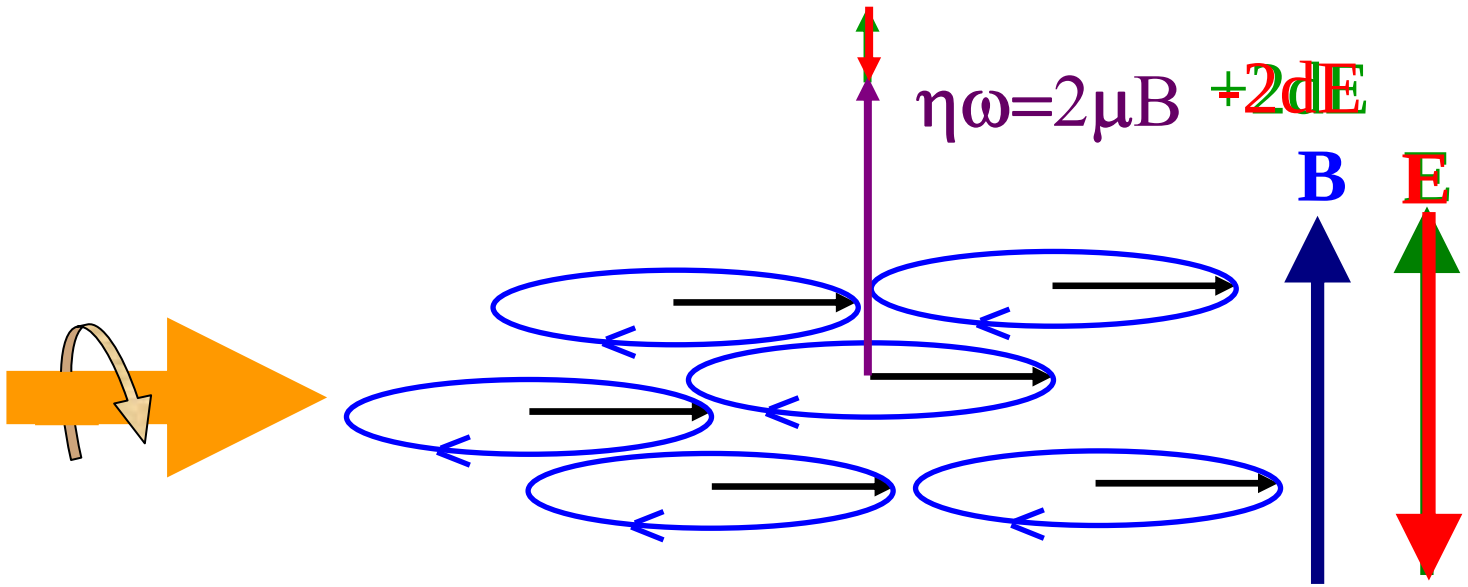
A. From cloud of accompanying “virtual” particles



Searching for new physics with the electron EDM



General method to detect an EDM



Energy level picture:

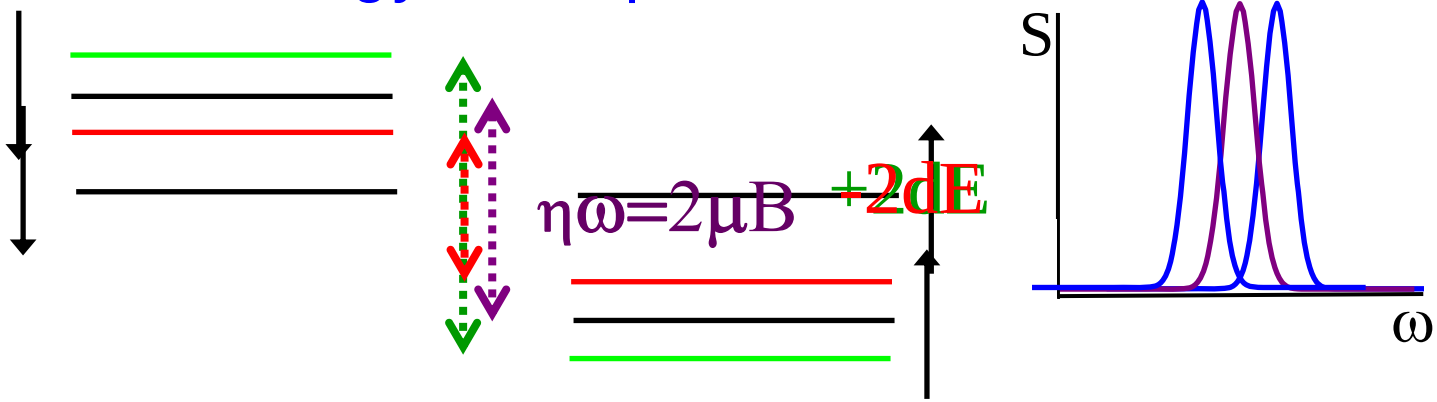
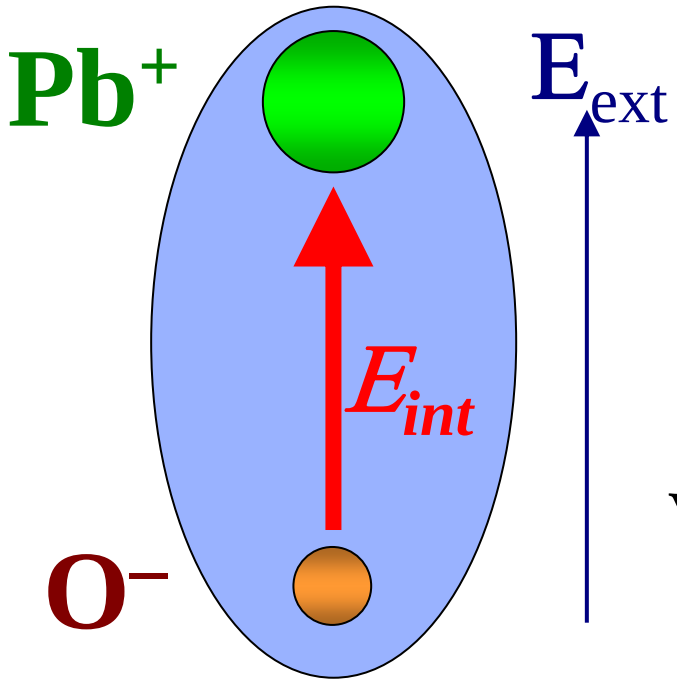


Figure of merit:

$$\frac{shift}{resolution} = \frac{dE}{(1/\tau_{coh})(S/N)^{-1}} \propto E \cdot \tau_{coh} \cdot \sqrt{\dot{N} \cdot T_{\text{int}}}$$

Amplifying the electric field E with a polar molecule



Electrical polarization of molecule subjects valence electrons to huge internal field

$E_{int} > 10^{10}$ V/cm

with modest polarizing field

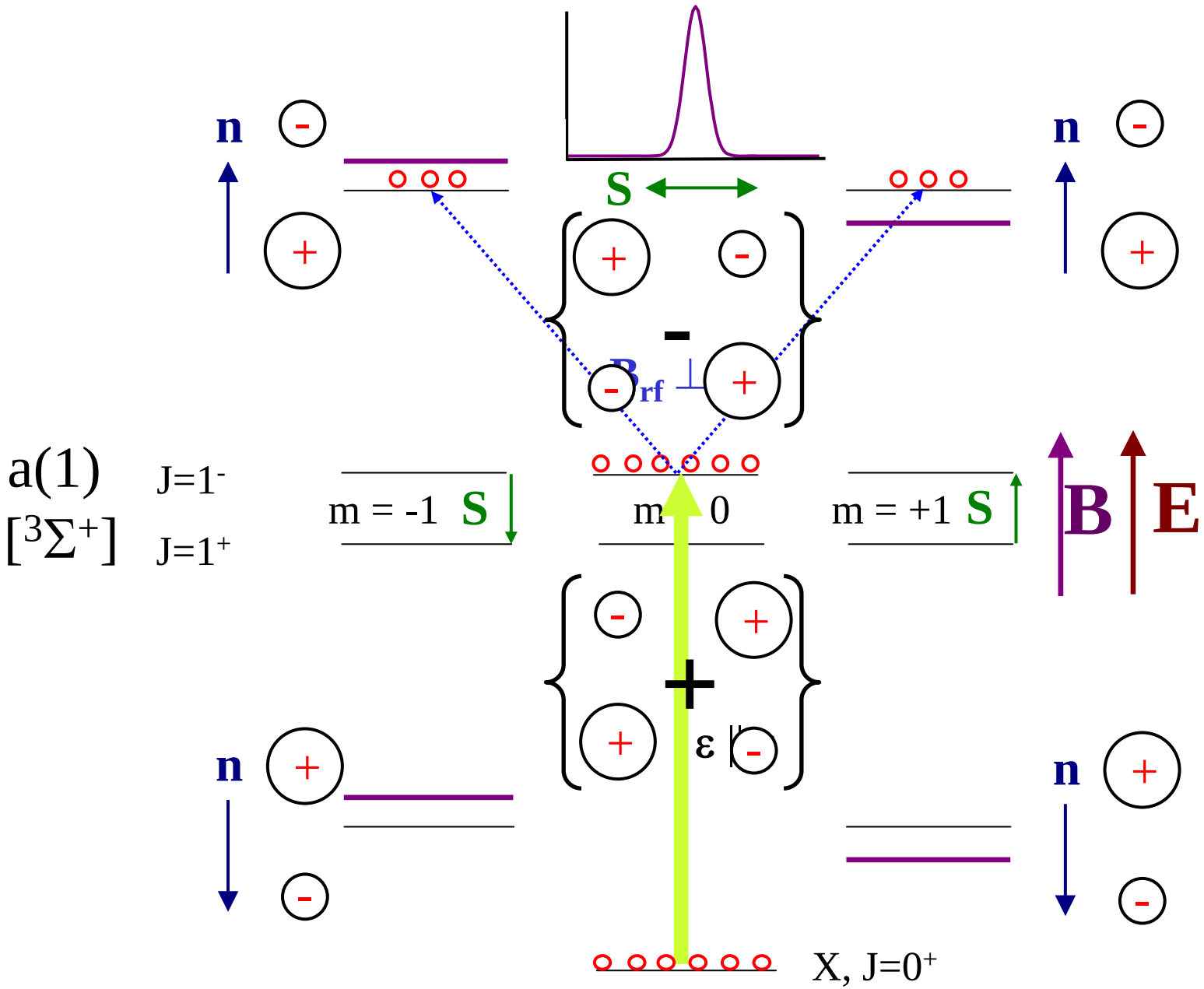
$E_{ext} \sim 10$ V/cm

Explicit calculations indicate valence electron feels

$E_{int} \sim \alpha^2 Z^3 \, e/a_0^2 \sim 2.1 - 4.0 \times 10^{10}$ V/cm **in PbO***

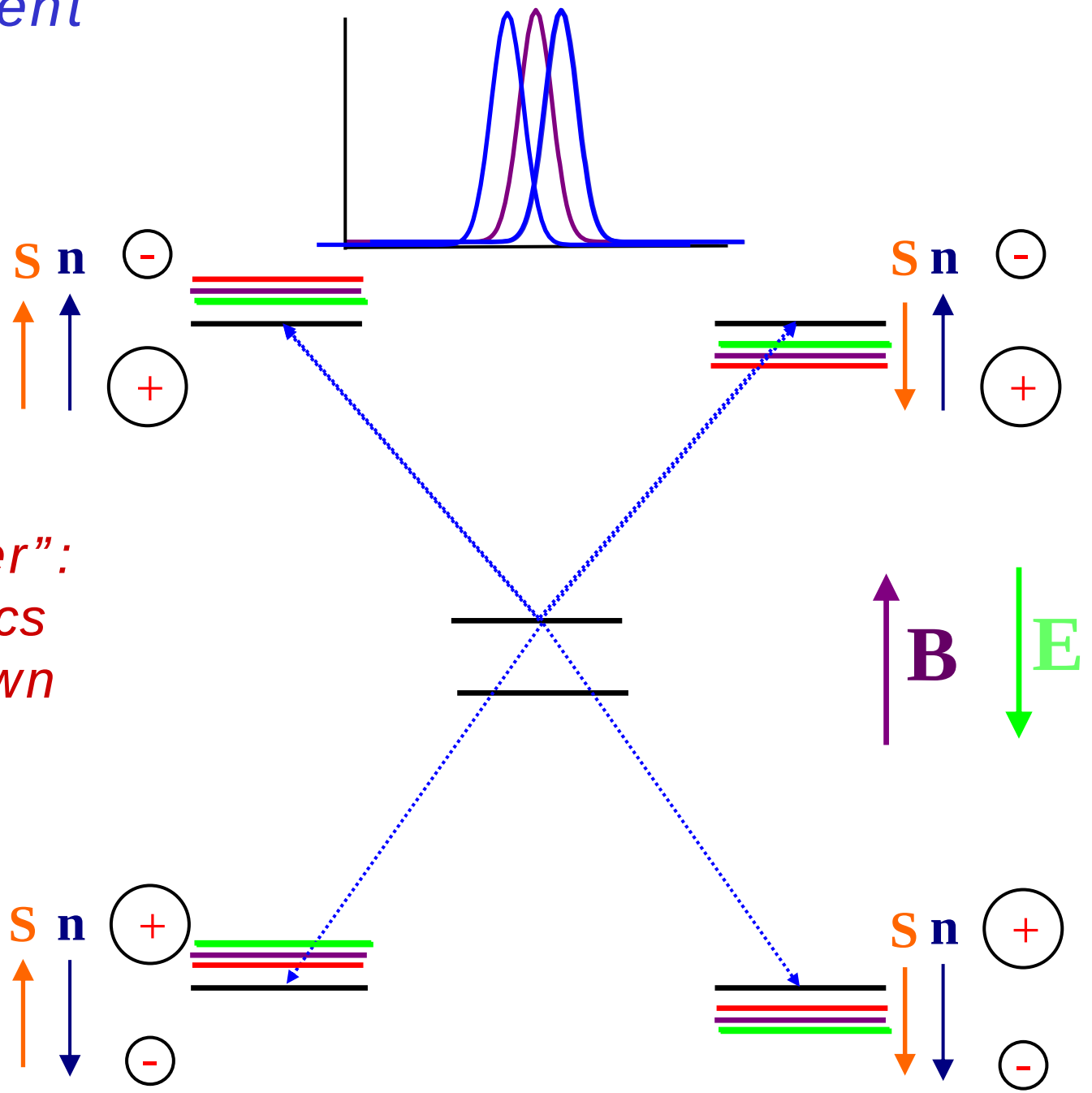
semiempirical: M. Kozlov & D.D., PRL **89**, 133001 (2002);
ab initio: Petrov, Titov, Isaev, Mosyagin, D.D., PRA **72**, 022505 (2005).

Spin alignment & molecular polarization in PbO (no EDM)



*EDM measurement in PbO**

"Internal co-magnetometer": most systematics cancel in up/down comparison!



The central dogma of physics (c.f. S. Freedman)

Theorist :: Experimentalist :: Fact

●

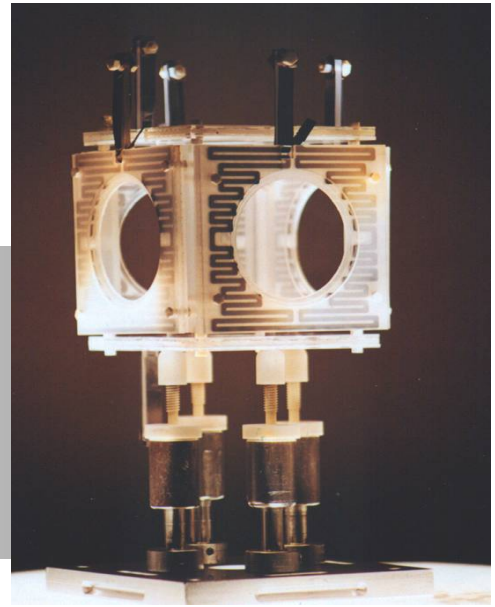
●

Farmer :: Pig :: Truffle

PbO vapor cell and oven

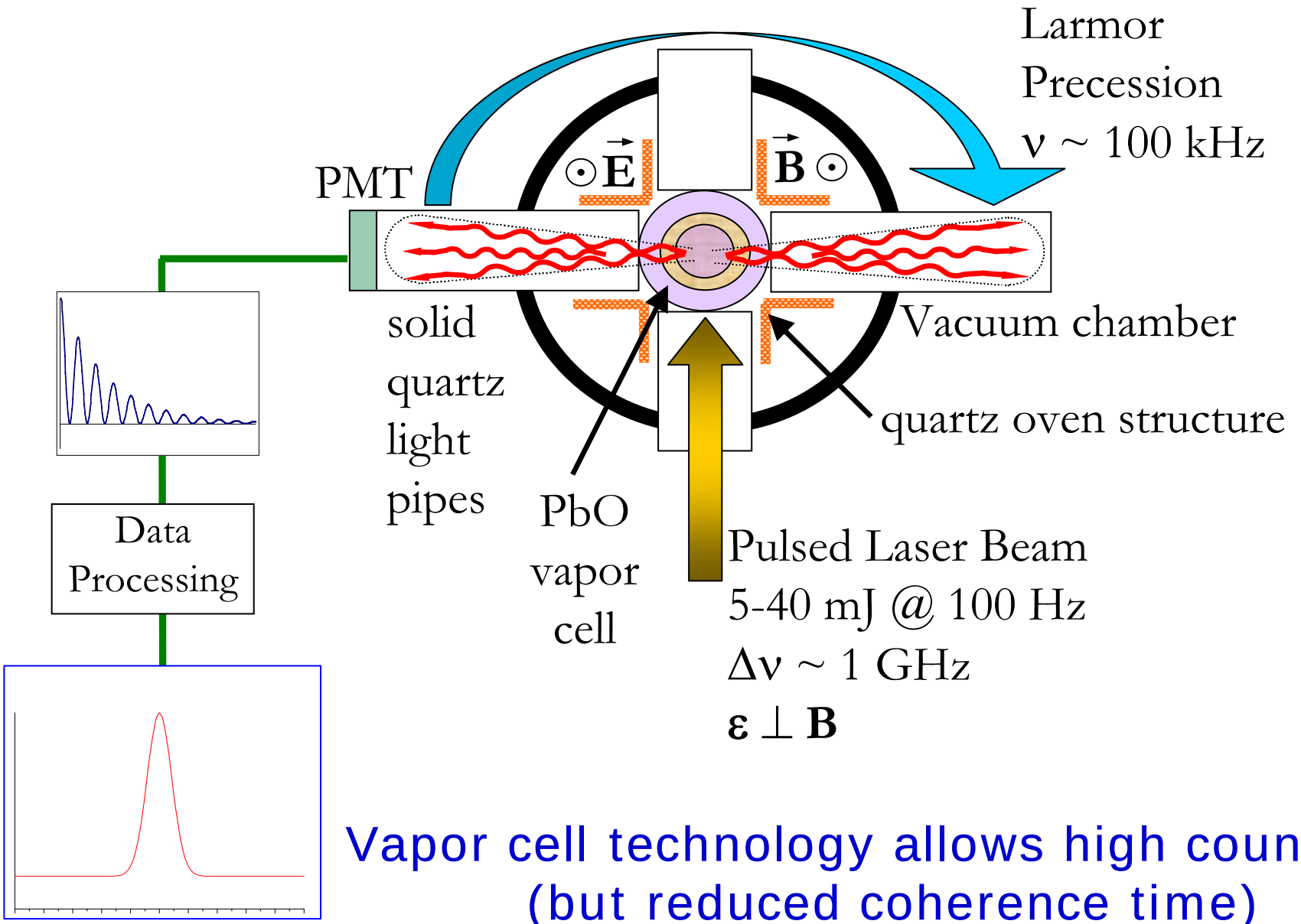
Sapphire windows bonded to ceramic frame with gold foil "glue"

Gold foil electrodes and "feedthroughs"



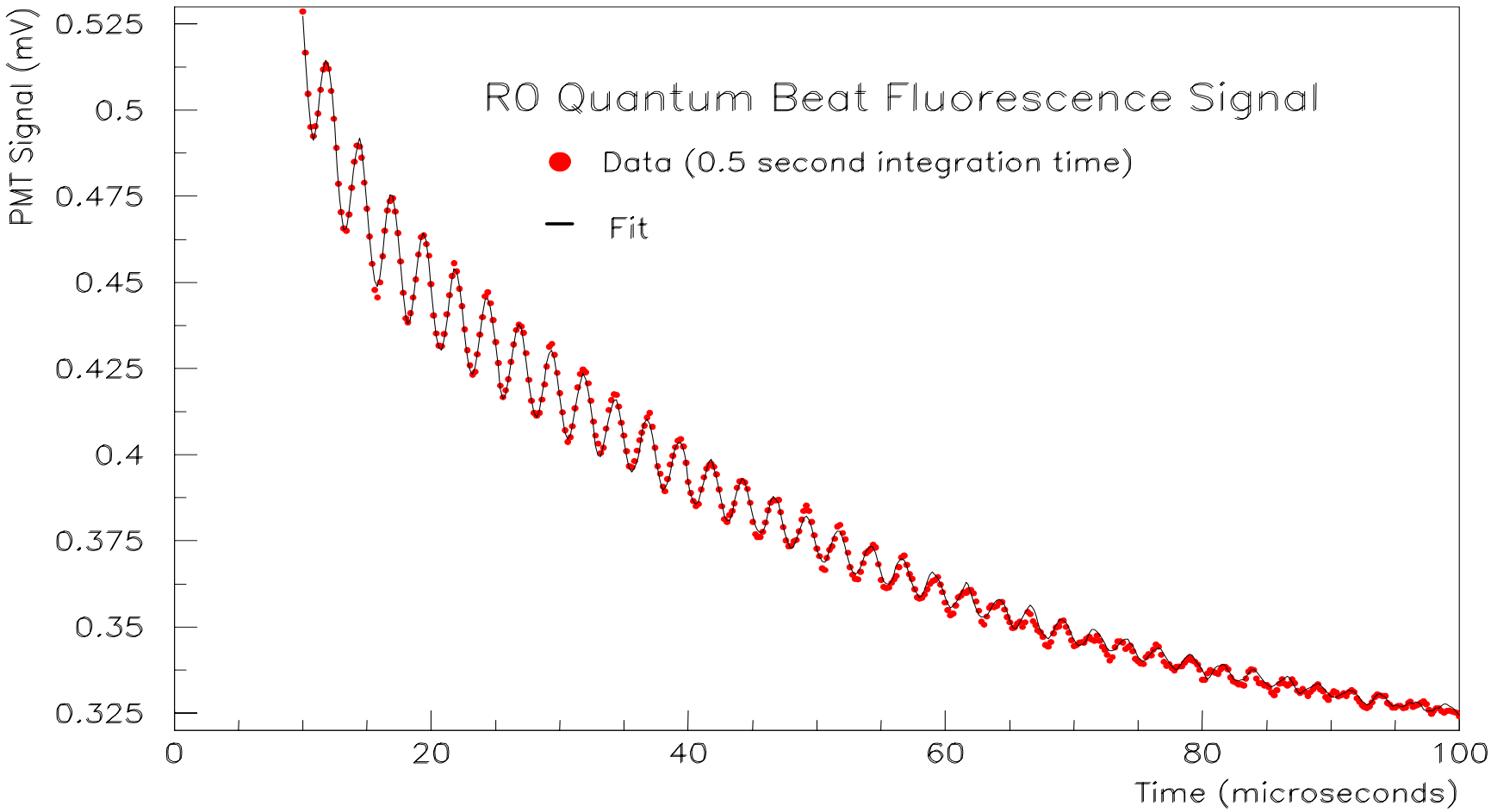
quartz oven body
800 C capability
wide optical access
w/non-inductive heater
for fast switching

Present Experimental Setup (top view)



Vapor cell technology allows high count rate
(but reduced coherence time)

Zeeman quantum beats in PbO



Excellent fit to Monte Carlo w/PbO motion, known lifetime

Shot noise-limited S/N in frequency extraction

(Laser-induced spin alignment only here)

Current status: a proof of principle

[D. Kawall *et al.*, PRL **92**, 133007 (2004)]

•PbO vapor cell technology in place

•Collisional cross-sections as expected ⇒anticipated density OK

•Signal sizes large, consistent with expectation;
improvements under way should reach target count rate: 10^{11}/s.

•Shot-noise limited frequency measurement
using quantum beats in fluorescence

•g-factors of Ω-doublet states match precisely
⇒co-magnetometer will be very effective

•E-fields of required size applied in cell; no apparent problems

⇒ First useful EDM data ~early 2006;
$\delta d_e \sim 3\times10^{-29}$ e·cm within ~2 years…?

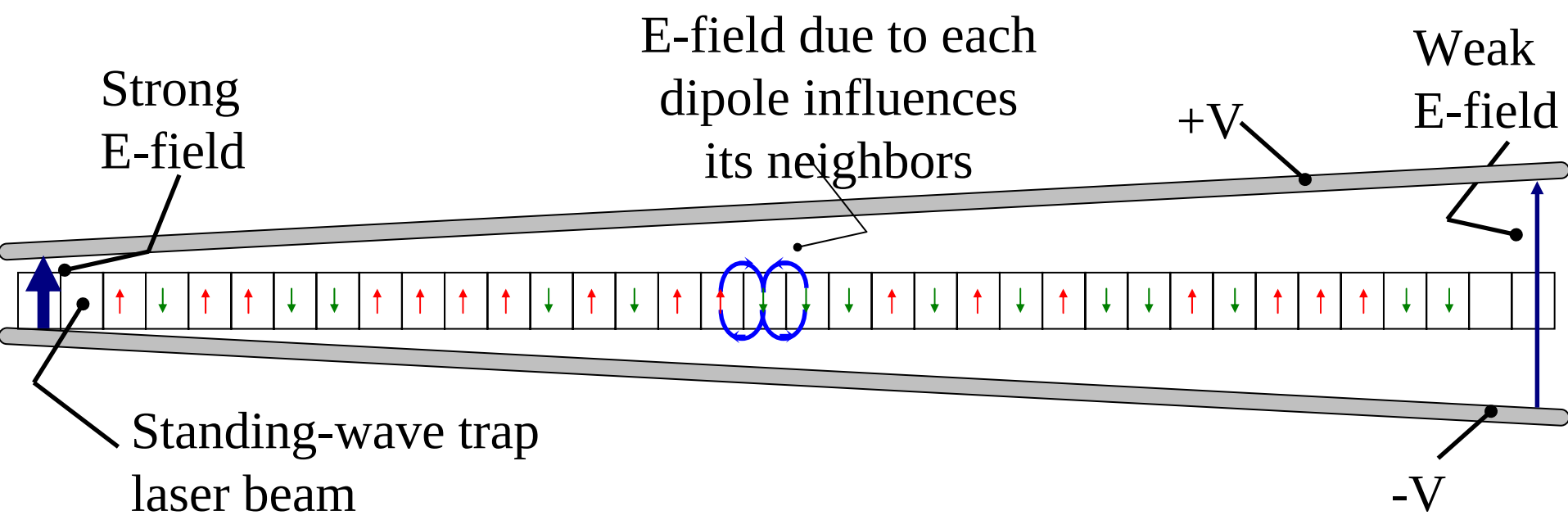
Applications of ultracold polar molecules

- Precision measurements/symmetry tests: narrow lines improve sensitivity & molecular structure *enhances* effects (small energy splittings)
  - →Time-reversal violating electric dipole moments *($\times 10^3$ vs. atoms)*
  - →Parity violation: properties of Z^0 boson & nuclear anapole moments *($\times 10^{11}$!!)*
  - →New tests of time-variation of fundamental constants? *($\times 10^3$ vs. atoms)*

- Coherent/quantum molecular dynamics
  - →Novel collisional phenomena (e.g. ultra-long range dimers)
  - →ultracold chemical reactions (e.g. tunneling through reaction barriers)

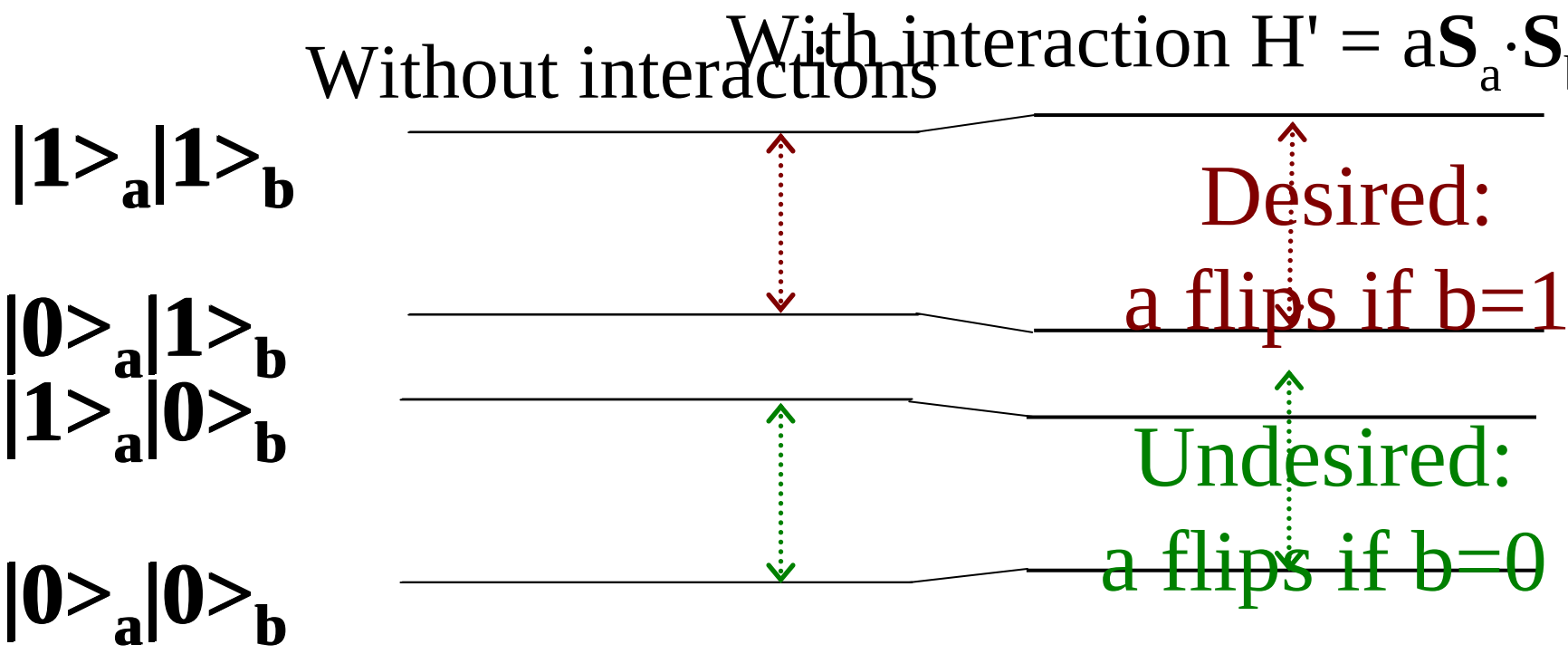
- Electrically polarized molecules have **tunable** interactions that are extremely strong, long-range, and anisotropic--*a new regime*
  - →Models of strongly-correlated systems (quantum Hall effect, etc.)
  - →Finite temperature quantum phase transitions
  - →New, exotic quantum phases (supersolid, checkerboard, etc.)
  - →novel BCS pairing mechanisms (models for exotic superconductivity)
  - →Large-scale quantum computation *D. DeMille, Phys. Rev. Lett **88**, 067901 (2002)*

Quantum computation with ultracold polar molecules



- bits = electric dipole moments of polarized diatomic molecules
- register = regular array of bits in “optical lattice” trap (weak trap ⇒low temp needed!)
- processor = rf resonance w/spectroscopic addressing (robust, like NMR)
- interaction = *electric* dipole-dipole (CNOT gate speed ~ 1-100 kHz)
- decoherence = scattering from trap laser (T ~ 5 s ⇒ N_{op} ~ 10^4-10^6 !)
- readout = laser ionization or cycling fluorescence + imaging (fairly standard)
- scaling up? (10^4- 10^7 bits looks reasonable: one/site via Mott insulator transition)

CNOT requires bit-bit interactions



Size of interaction term “a”
determines maximum gate speed:
$\tau^{-1} \sim \Delta\nu \sim a$

Quantum computation with trapped polar molecules

- Quantum computer based on ultracold polar molecules in an optical lattice trap can plausibly reach $>10^4$ bits and $>10^4$ operations in ~5 s decoherence time

- Based heavily on existing work & likely progress:

  Main requirement is sample of ultracold ($T \sim 10\ \mu K$) polar molecules with phase space density ~10^{-3}

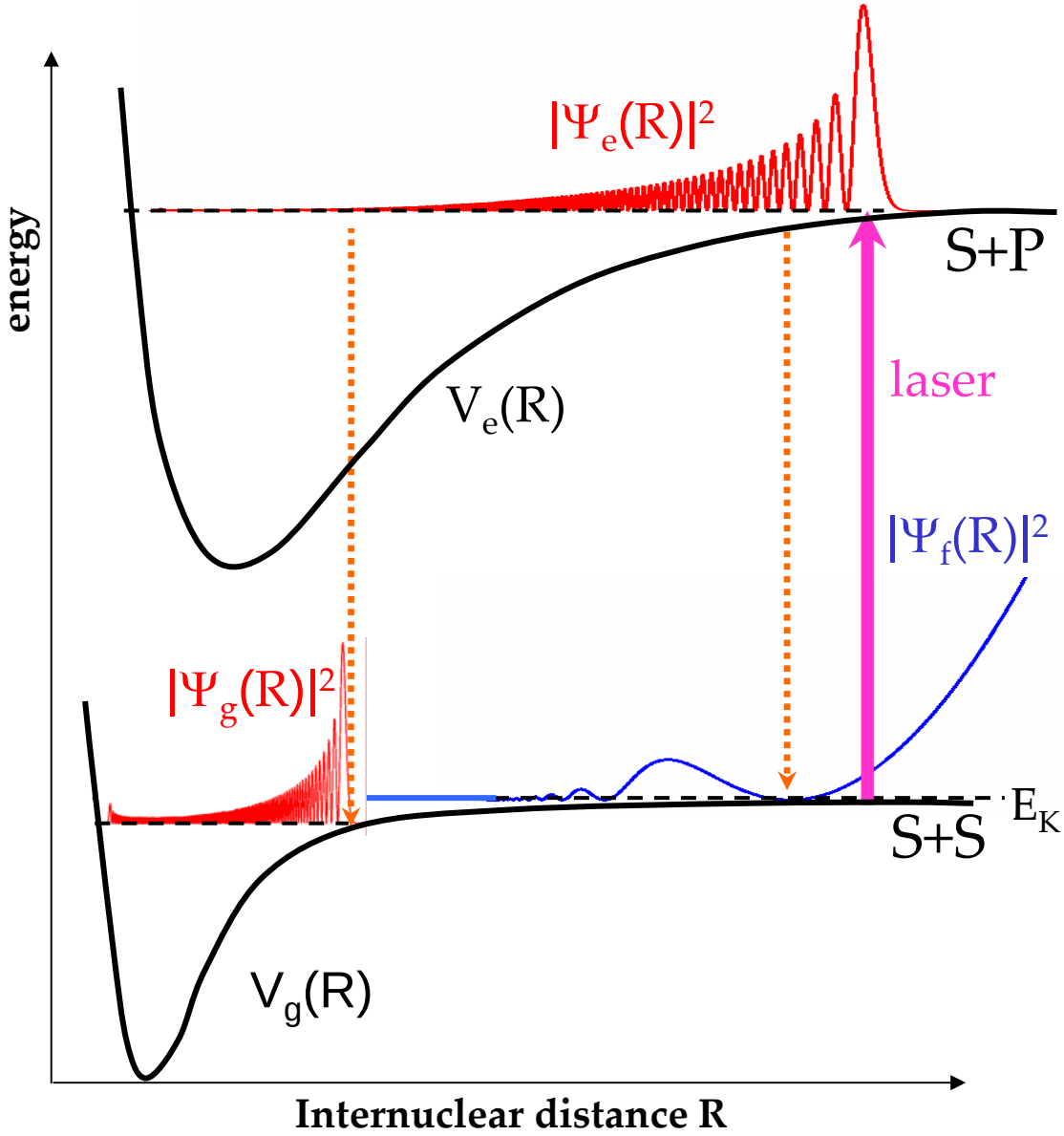
- Anticipated performance is above some very significant technological thresholds:

$N_{op} > 10^4 \Rightarrow$ *robust* error correction OK?

Crude scaling $\Rightarrow$

300 bits, 10^4 ops/s $\approx$ *teraflop* classical computer

Cold molecules from cold atoms: photoassociation

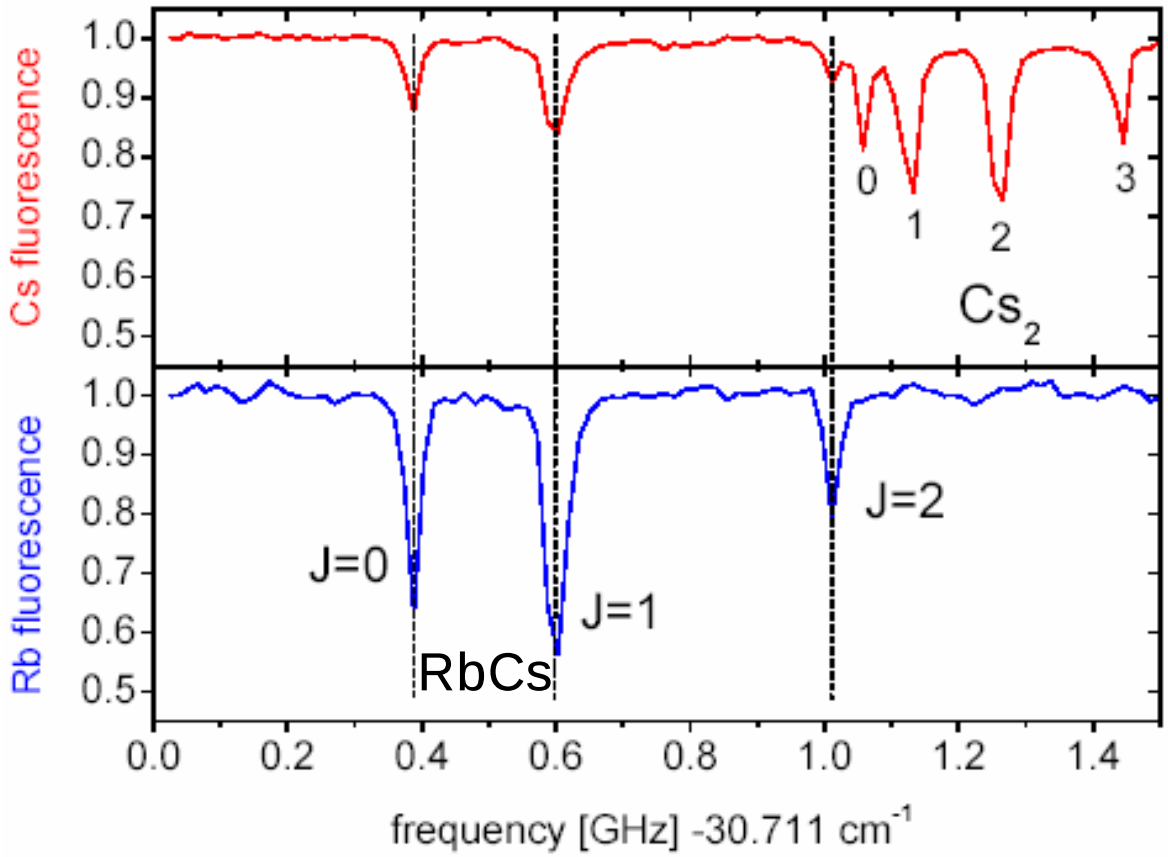


- very weak free-bound (but excited) transition driven by laser for long times (trapped atoms)
- electronically excited molecules decay to hot free atoms *or* to ground-state molecules
- Production of *polar* molecules requires assembly from two different atomic species
- molecules can be formed in single rotational state, at translational temperature of atoms (100 μK routine, =1 μK possible)

BUT molecules are formed in range of high vibrational states

MOT trap loss photoassociation spectra

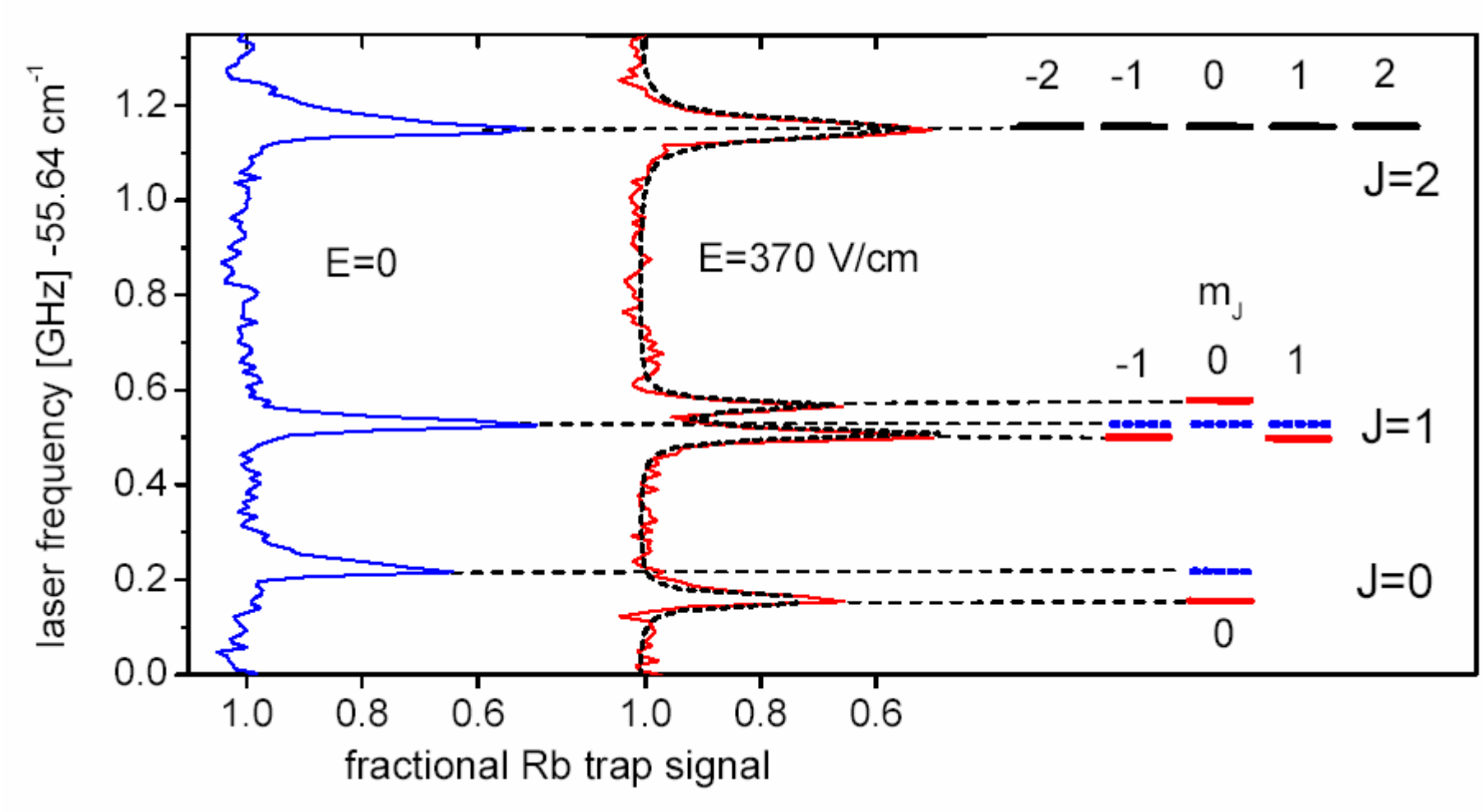
RbCs* and Cs_2* formation ($\Omega = 0$)



- up to 70% depletion of trap for RbCs $\Rightarrow$ near 100% atom-molecule conversion
- spectroscopically selective production of individual low-J rotational states

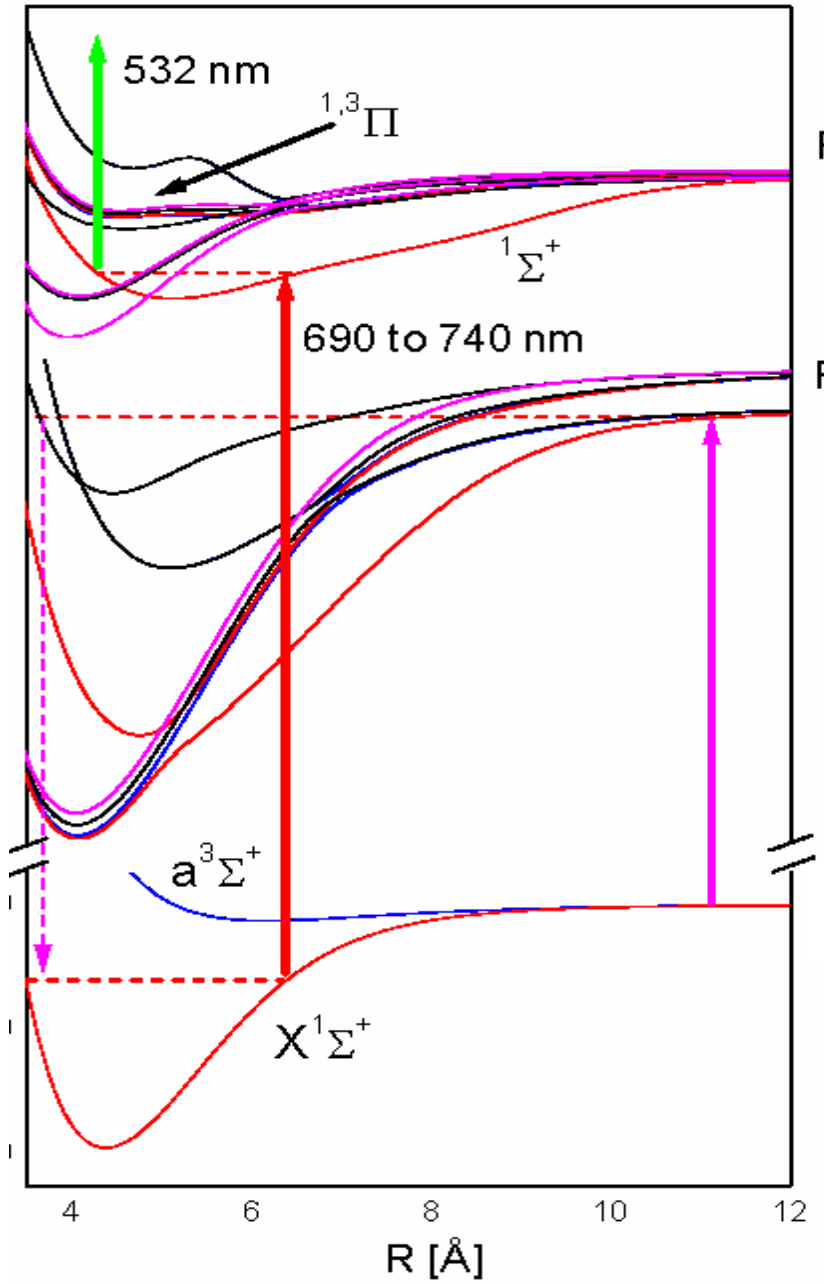
A.J. Kerman *et al.*, Phys Rev. Lett. **92**, 033004 (2004)

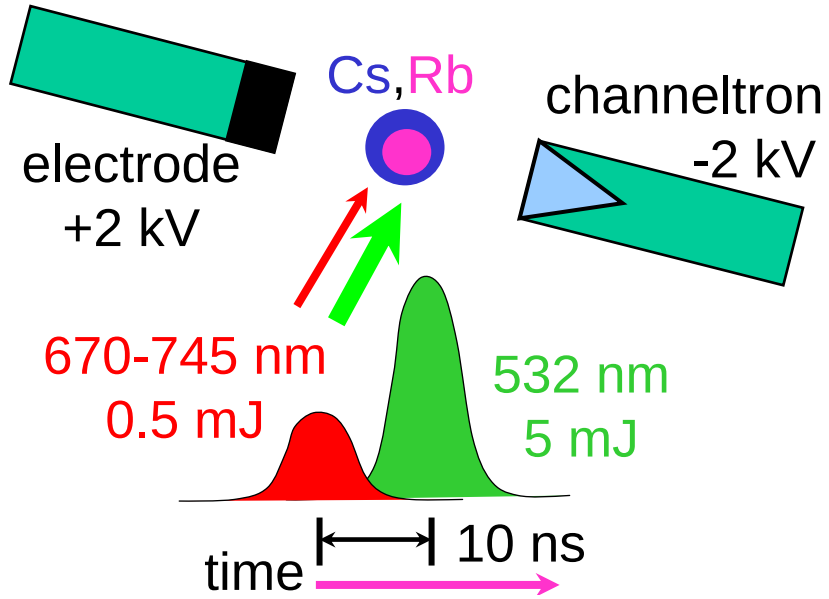
Verification of polar molecules: behavior in E-field

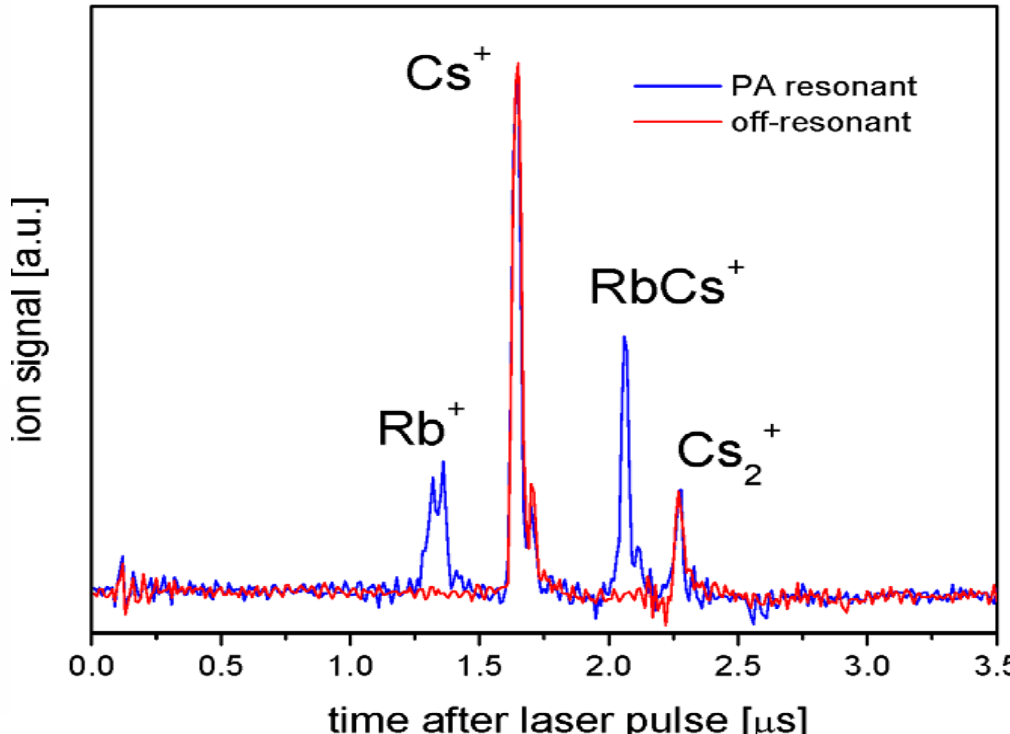


Fitted electric dipole moment for this ($\Omega=0^+$) state: μ = 1.3 Debye

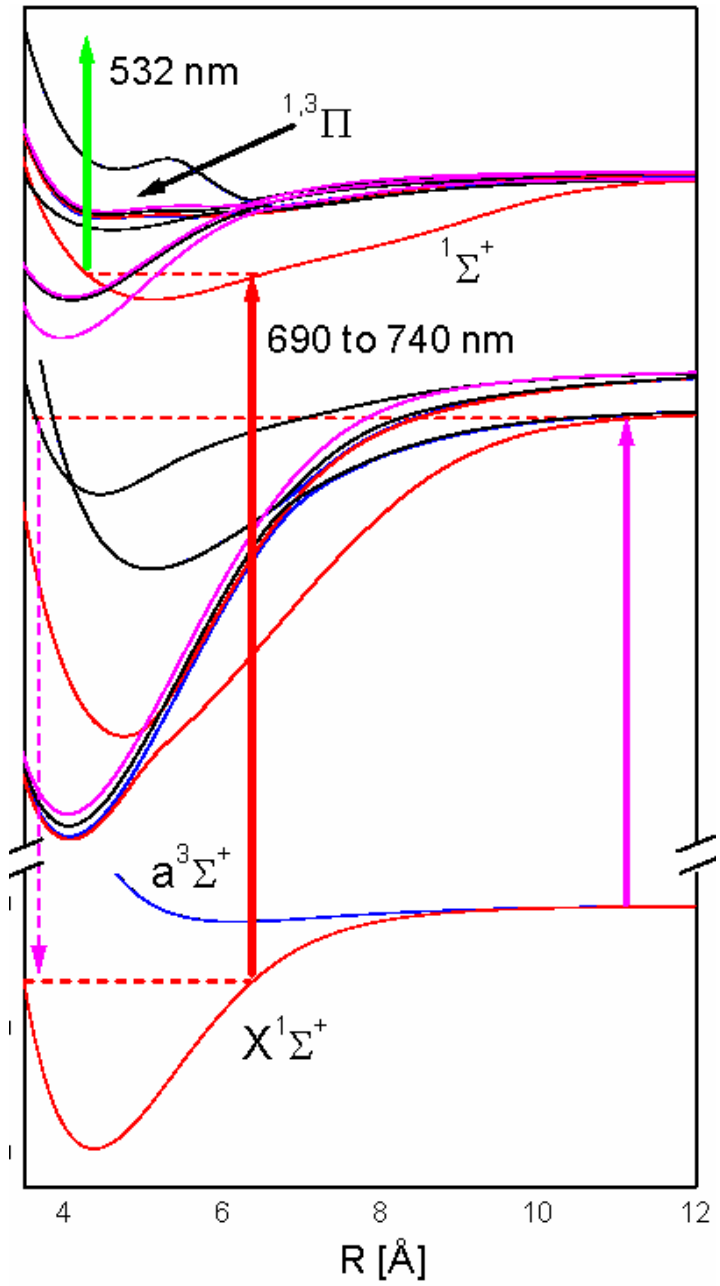
Detection of vibrationally excited RbCs

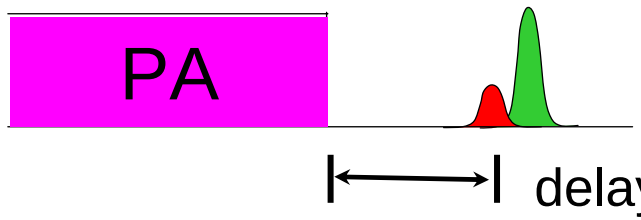


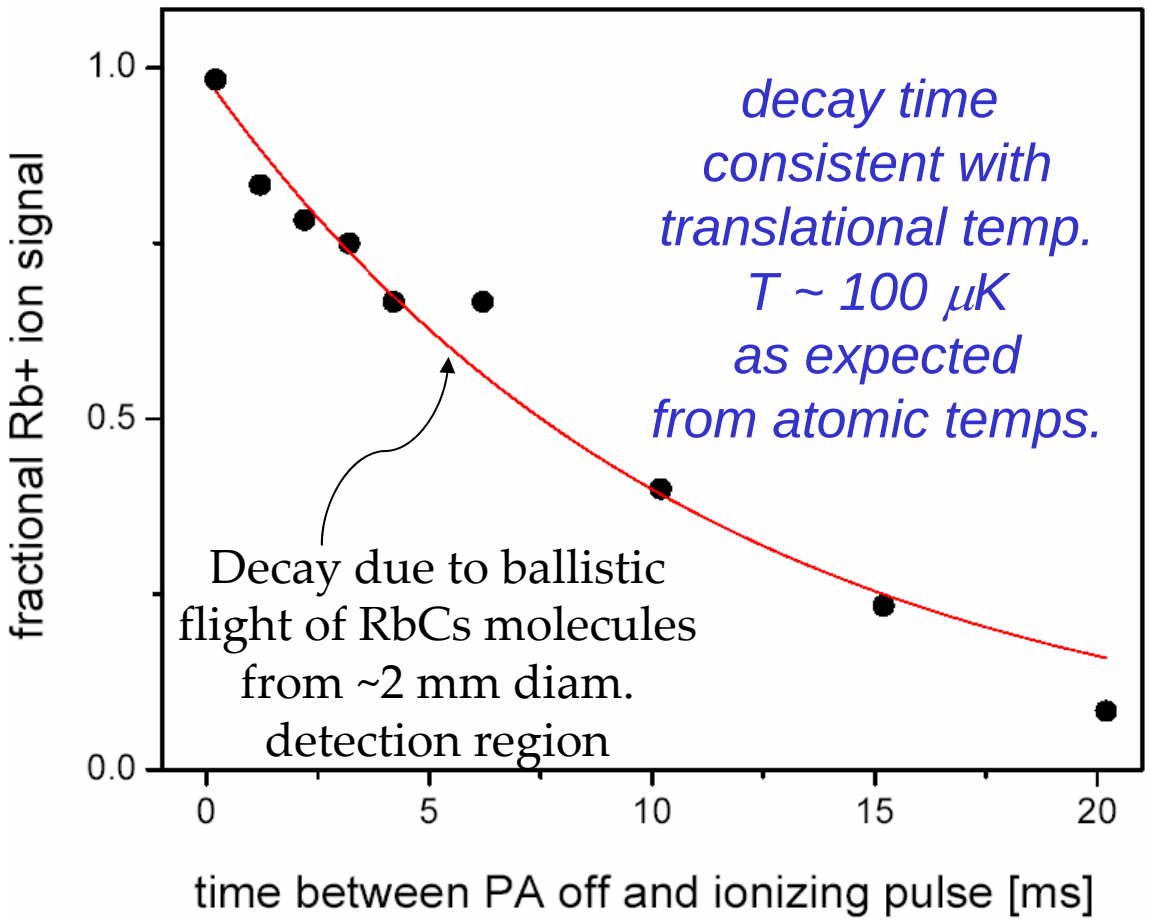




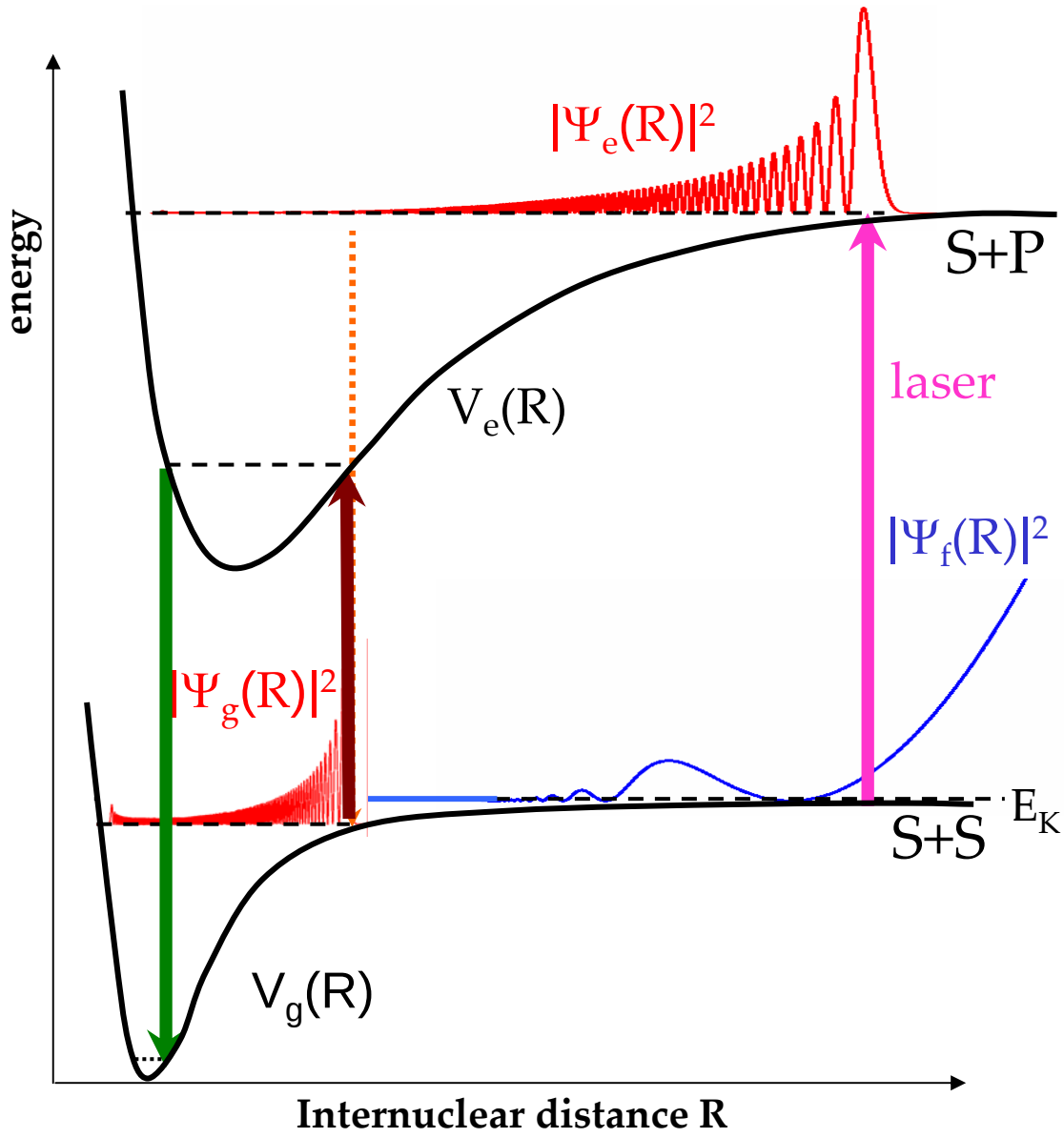
Vibrationally excited RbCs @T = 100 μK







Cold molecules from cold atoms: stopping the vibration



- free-bound (but excited) transition driven by laser

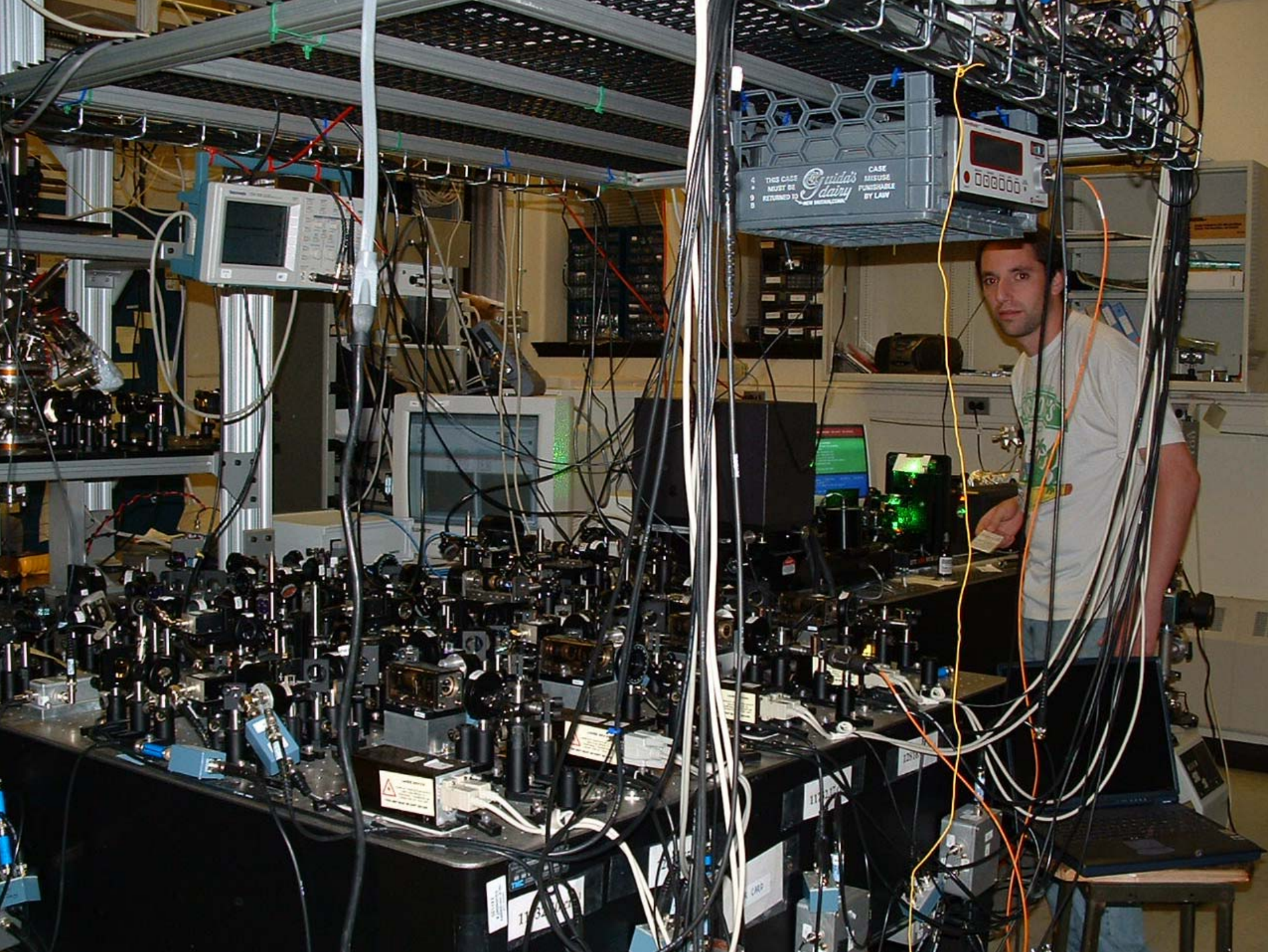
- excited molecules can decay to molecular ground state

- molecules can be formed in single rotational state, at translational temperature of atoms (100 μK routine, =1 μK possible) *BUT molecules are formed in range of high vibrational states*

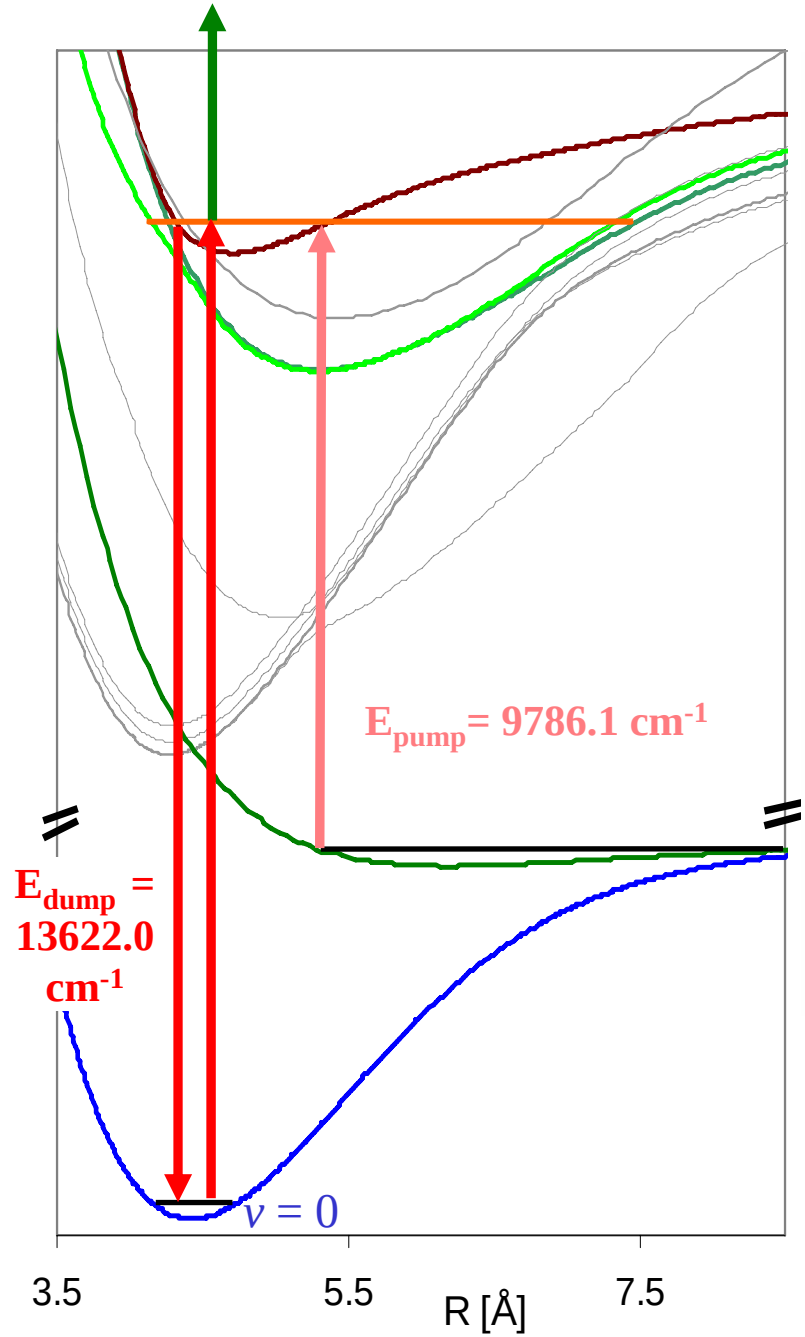
- High vibrational states are *UNSTABLE* to collisions and have *NEGLIGIBLE POLARITY* ⇒need vibrational ground state!

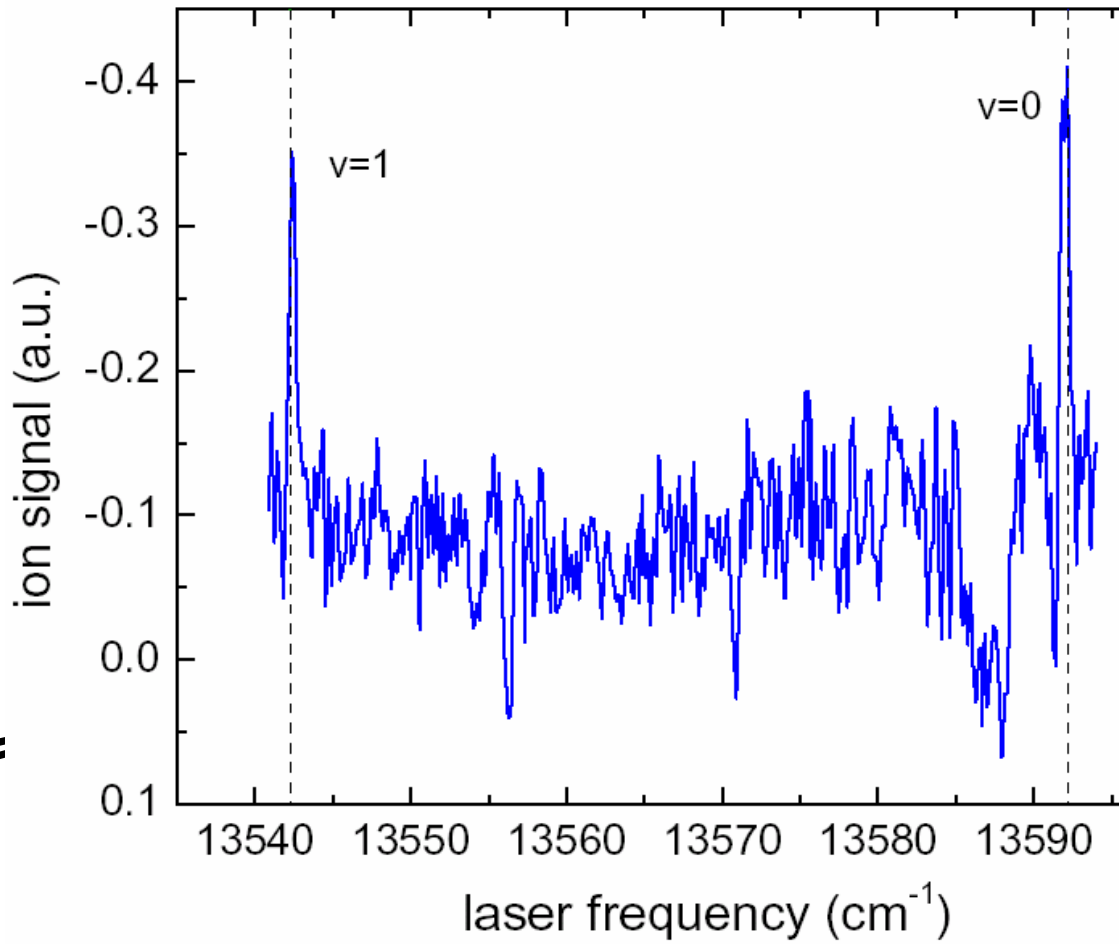
- Laser pulses should be able to transfer one excited state to vibrational ground state:

⇒TRULY ultracold molecules (translation, rotation, vibration)


THIS CASE MUST BE RETURNED TO
Guida's dairy
CASE MISUSE PUNISHABLE BY LAW

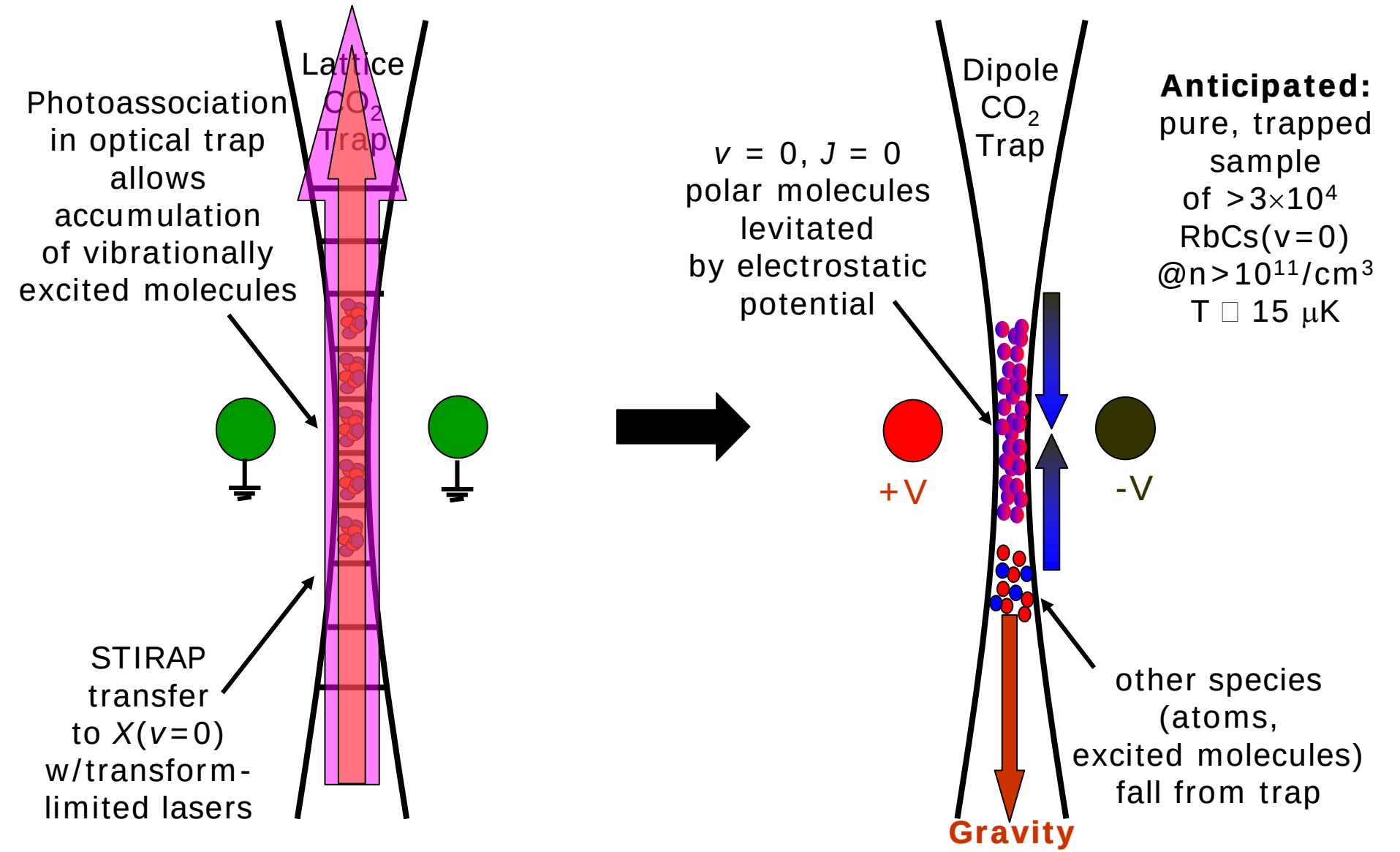
Production of absolute ground state molecules





- Raman transfer verified on ~6 separate transitions
- Estimated efficiency ~8%, limited by poor pulsed laser spectral profiles

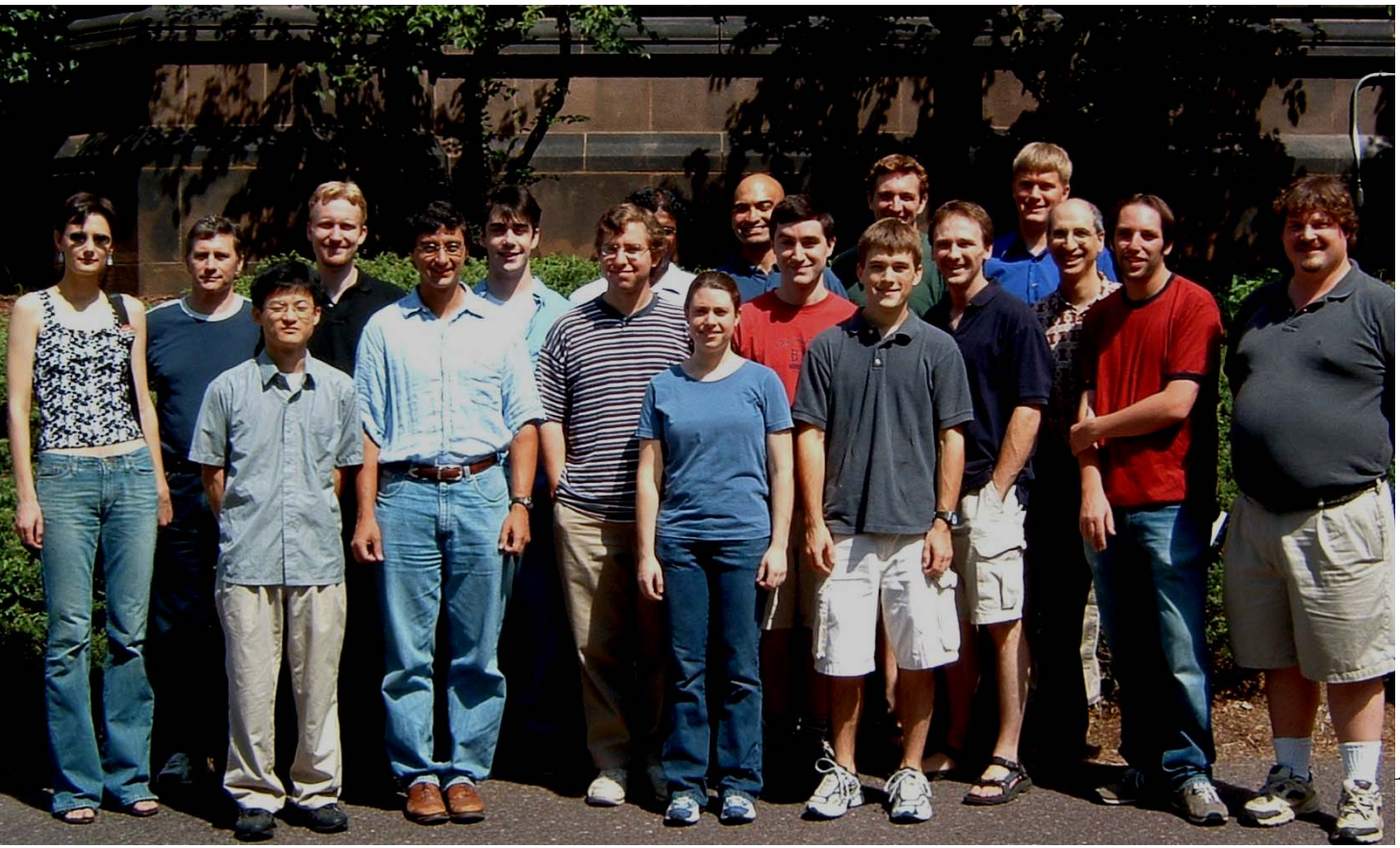
Coming next: "distilled" sample of polar, absolute ground-state RbCs molecules



Status & Outlook: ultracold polar molecules

- Optical production of ultracold polar molecules now in hand!
  [J.Sage et al., PRL **94**, 203001 (2005)]
  T ~ 100 μK now, but obvious route to lower temperatures
- Formation rates of up to ~10^7 mol/s/level in high vibrational states
  AND
  efficient transfer to v=0 ground state (~5% observed, 100% possible)
  ⇒ Large samples of stable, ultracold polar molecules in reach
- molecule trapping (CO_2 lattice/FORT),
  collisions & manipulation (E-fields, rotational transitions, etc.)
  are next
- Ultracold polar molecules are set to open new frontiers in
  many-body physics, precision measurements, & chemical physics

DeMille Group



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