

# Exploring Fundamental Physics: The Electric Dipole Moment of the Electron

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# A Question at Large Scale

## What “Happened” to Antimatter ?

- *Matter* and *antimatter* particles are created (and annihilated) in pairs.
- A tiny portion of *matter*, about one particle per billion, managed to survive the Big Bang.  
→ Baryon Asymmetry Problem of the Universe (BAU)
- Fundamental **symmetry violation** could be at the heart of this problem.

# A Possible Explanation Via: Sakharov's Conditions<sup>1</sup>

Condition 1: Distinguished direction of time (time arrow)  
Departure from thermal equilibrium

Condition 2: *Baryon number* ( $A$ ) violation  
Inflation suggests that universe started with  $A = 0$

Condition 3:  $(\mathcal{CP})$ -violating physics present  
Standard Model  $(\mathcal{CP})$  violation is regarded as insufficient  
(SM-Baryogenesis, SM-Leptogenesis?)

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<sup>1</sup>M. Dine, A. Kusenko, "Origin of the matter-antimatter asymmetry", *Rev. Mod. Phys.* **76** (2004) 1

# Fundamental Discrete Symmetries

A bit of safe ground ?

$\mathcal{CPT}$  theorem:<sup>2</sup>  
Local QFTs invariant

One example: The free Dirac equation (Weyl notation)

$$\begin{aligned} \hat{\mathcal{K}}^\dagger \hat{\mathcal{P}}^\dagger \hat{\mathcal{C}}^\dagger (-i\hbar\gamma^\mu \partial_\mu + m_0 c^2 \mathbb{1}_4) \hat{\mathcal{C}} \hat{\mathcal{P}} \hat{\mathcal{K}} \hat{\mathcal{K}}^\dagger \hat{\mathcal{P}}^\dagger \hat{\mathcal{C}}^\dagger \underline{\Psi}(x) &= 0 \\ (\gamma^3)^\dagger (\gamma^1)^\dagger \hat{K}_0 \gamma^0 i(\gamma^2)^\dagger \hat{K}_0 (-i\hbar\gamma^\mu \partial_\mu + m_0 c^2 \mathbb{1}_4) i\gamma^2 \hat{K}_0 \gamma^0 \gamma^1 \gamma^3 \hat{K}_0 \\ (\gamma^3)^\dagger (\gamma^1)^\dagger \hat{K}_0 \gamma^0 i(\gamma^2)^\dagger \hat{K}_0 \underline{\Psi}(x) &= 0 \\ (-i\hbar\gamma^\mu \partial_\mu + m_0 c^2 \mathbb{1}_4) \underline{\Psi}(x) &= 0 \end{aligned}$$

- $\mathcal{CPT}$  invariance is connected to Lorentz invariance
- We have good reasons to “believe” in  $\mathcal{CPT}$  symmetry

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<sup>2</sup>R. F. Streater, A. S. Wightman, “*PCT, Spin and Statistics, and All That*”

# Fundamental Discrete Symmetries

Individual/combined symmetries may be violated

- The fall of  $\mathcal{P}$  invariance<sup>3</sup>

$$\begin{array}{ccc} \pi^+ \rightarrow \mu^+ + \nu_\mu & \xrightarrow{\hat{\mathcal{P}}} & \pi^+ \rightarrow \mu^+ + \nu_\mu \\ \text{both left-handed helicity} & & \text{both right-handed helicity (impossible)} \\[10pt] \pi^+ \rightarrow \mu^+ + \nu_\mu & \xrightarrow{\hat{\mathcal{C}}\hat{\mathcal{P}}} & \pi^- \rightarrow \mu^- + \bar{\nu}_\mu \\ \text{both left-handed helicity} & & \text{both right-handed helicity (possible)} \end{array}$$

Perhaps it is  $(\mathcal{CP})$  that is always conserved ?

- The fall of  $(\mathcal{CP})$  invariance<sup>4</sup>

$$K_2 = \frac{1}{\sqrt{2}} (K_0 + \overline{K}_0) \rightarrow \pi + \pi$$

is  $(\mathcal{CP})$ -odd, about 0.2% of events.

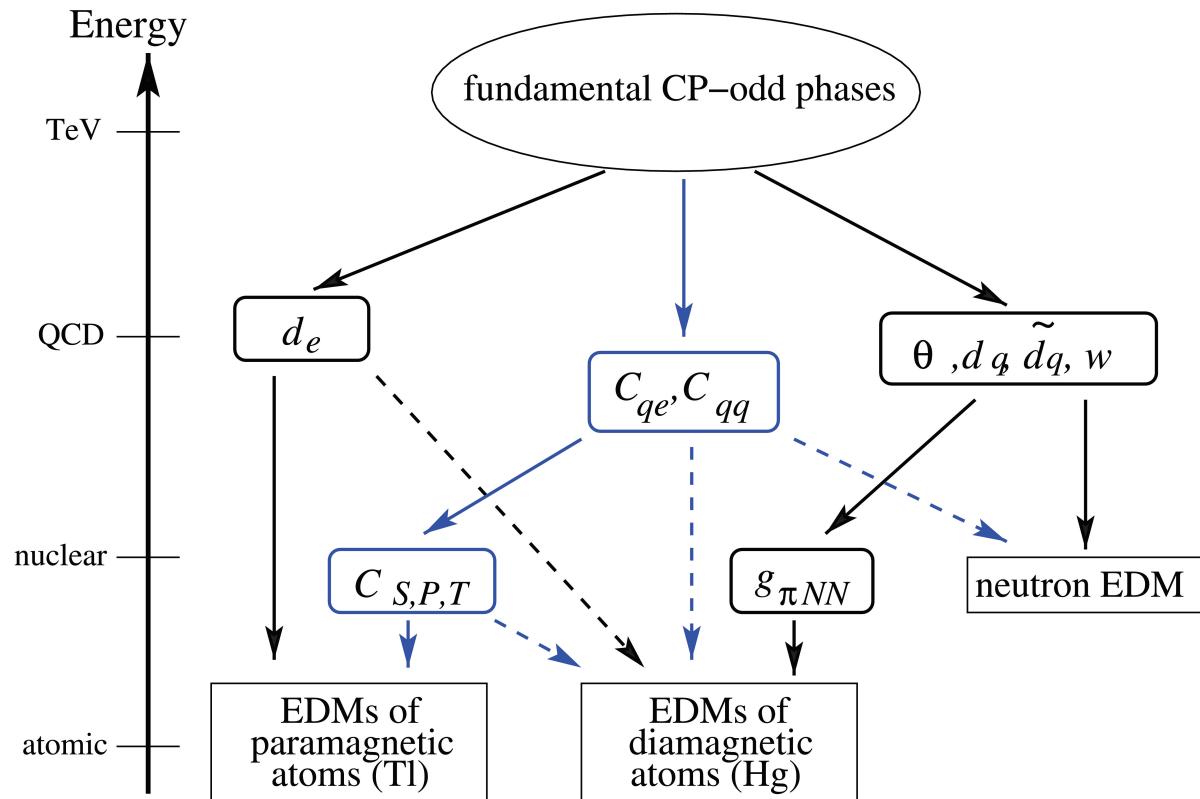
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<sup>3</sup>C. S. Wu et al., *Phys Rev* **105** (1957) 254

<sup>4</sup>J. H. Christenson et al., *Phys Rev Lett* **13** (1964) 138

# Electric Dipole Moment of Paramagnetic Atoms/Molecules

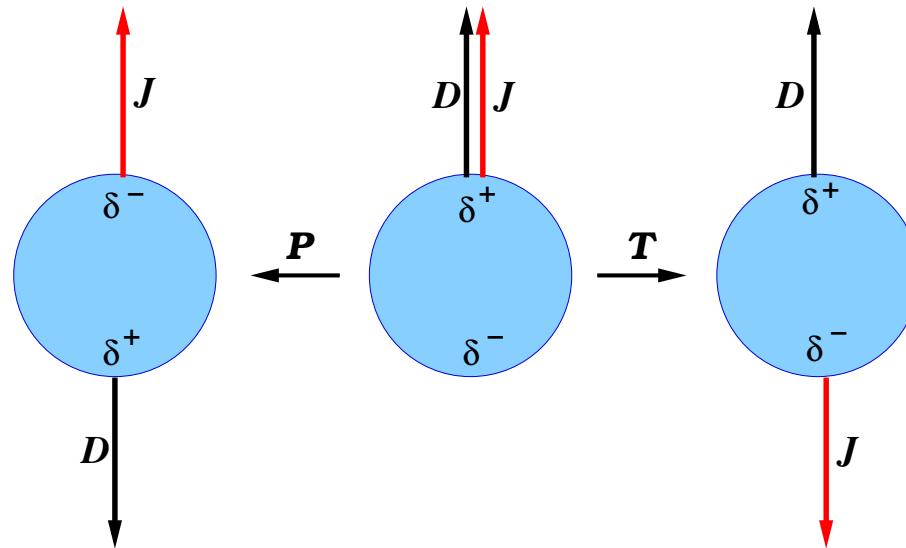
## Possible sources<sup>5</sup>



1. Intrinsic EDM of an electron
2. ( $\mathcal{P}$  and  $\mathcal{T}$ ) violating electron-nucleon interaction

<sup>5</sup>M. Pospelov, A. Ritz, "Electric dipole moments as probes of new physics", *Ann. Phys.* **318** (2005) 119

# Testing Time-Reversal Invariance: The Electron Electric Dipole Moment ( $e$ EDM) $\vec{D}$



$\vec{D}$  and  $\vec{J}$  (anti-)collinear,  $\leftarrow$  Pauli exclusion principle<sup>6</sup>

Implies violation of **Parity**( $\mathcal{P}$ ) and **Motion-Reversal**( $\mathcal{T}$ ) symmetries<sup>7</sup>

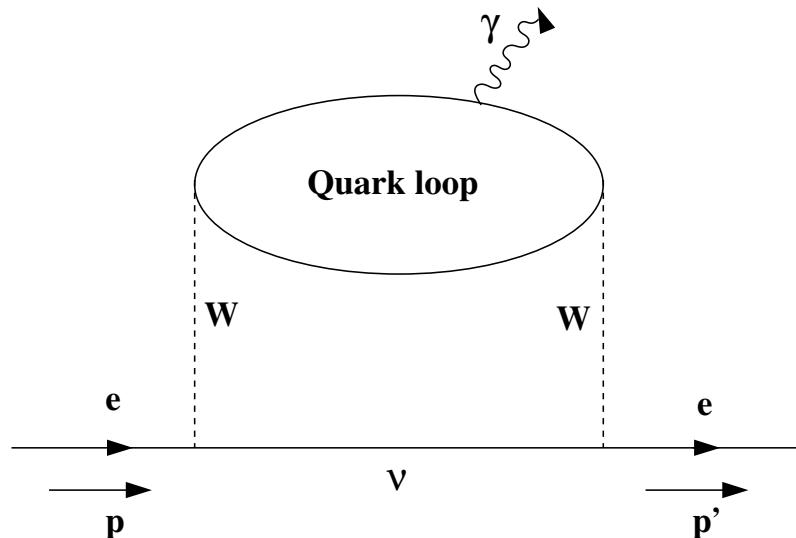
$\mathcal{CPT} \Rightarrow$  a kind of ( $\mathcal{CP}$ ) violating interaction

<sup>6</sup>Hunter, *Science* **252** (1991) 73

<sup>7</sup>T.D. Lee, C.N. Yang, *BNL* **443** (1957) T91

# The induced fermion EDM

## Standard Model Picture



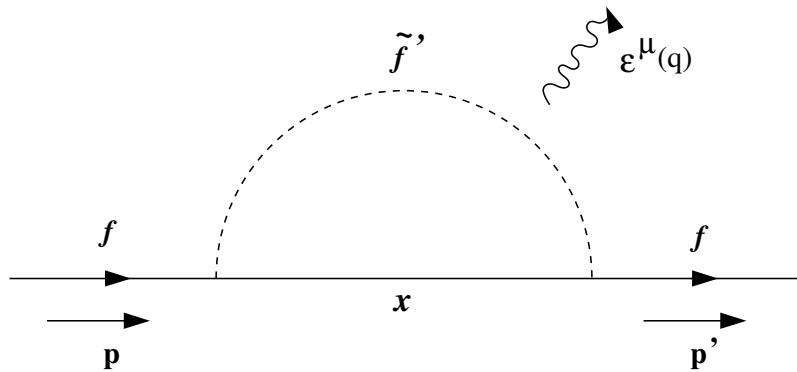
- Only  $\mathcal{CP}$  violation in the quark-mixing matrix (CKM)
- Electron only interacts indirectly via weak interaction with virtual quarks
- Such two-loop diagrams give zero  $\mathcal{CP}$ -odd contribution<sup>8</sup>
- Three-loop  $\mathcal{CP}$ -odd contributions zero in the absence of gluonic corrections<sup>9</sup>
- The standard-model prediction is immeasurably small:  
 $d_e^{SM} \leq 10^{-38} e \text{ cm}$

<sup>8</sup>E.D. Commins, *Adv At Mol Opt Phys* **40** (1998) 1

<sup>9</sup>M. Pospelov, I.B. Khriplovich, *Sov J Nuc Phys* **53** (1991) 638

# The induced fermion EDM

## Beyond the Standard Model



$\chi$ : chargino, neutralino

$\tilde{f}'$ : supersymmetry (s)-fermion

$\epsilon^\mu(q)$ : photon

Chargino ( $\tilde{\chi}_{1,2}^\pm$ ), neutralino ( $\tilde{\chi}_{1,2,3,4}^0$ ) or gluino ( $\tilde{g}^a$ ) fermion/sfermion interaction Lagrangian:

$$\mathcal{L}_{\chi f \tilde{f}'} = g_{Lij}^{\chi f \tilde{f}'_j} (\bar{\chi}_i P_L f) \tilde{f}'_j^* + g_{Rij}^{\chi f \tilde{f}'_j} (\bar{\chi}_i P_R f) \tilde{f}'_j^* + h.c.$$

One-loop fermion EDM:<sup>10</sup>

$$\left( \frac{dE}{e} \right)^\chi = \frac{m\chi_i}{16\pi^2 m_{\tilde{f}'_j}^2} \mathcal{I}m \left[ \left( g_{Rij}^{\chi f \tilde{f}'_j} \right)^* g_{Lij}^{\chi f \tilde{f}'_j} \right] \left[ Q_\chi A \left( \frac{m\chi_i}{m_{\tilde{f}'_j}^2} \right) + Q_{\tilde{f}'_j} B \left( \frac{m\chi_i}{m_{\tilde{f}'_j}^2} \right) \right]$$

MSSM (“naïve SUSY”) prediction:

$$d_e \leq 10^{-27} e \text{ cm}$$

<sup>10</sup>J. Ellis, J.S. Lee, A. Pilaftsis, *J High Energy Phys* **10** (2008) 049

# Search for the Electron EDM

$d_e$  from an atomic/molecular many-body problem

- Unpaired  $e^-$  in a stationary atomic/molecular state
- Measurement of an EDM dependent energy difference (transition energy)  $\Delta\epsilon_t$  of atomic/molecular quantum states.
- Theory determination of an **enhancement**<sup>11</sup>

$$d_e = \frac{\Delta\epsilon_t}{E_{\text{eff}}} \begin{array}{l} (\text{Experiment}) \\ (\text{Theory}) \end{array}$$

- Enhancement factor  $R$  “translates” between atomic and particle scales and is related to the **EDM effective electric field** at the position of the electron,

$$R \propto E_{\text{eff}}$$

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<sup>11</sup>P.G.H. Sandars, *J Phys B: At Mol Opt Phys* **1** (1968) 499

# Search for the Electron EDM

## Atomic/molecular enhancement

- In the **non-relativistic limit** the EDM expectation value vanishes:

$$\langle \hat{H}_{\text{EDM}} \rangle = 0$$

(Schiff's Theorem<sup>12</sup>)

- Relativistic view leads to a non-zero value, essentially due to length contraction in the observer frame<sup>13</sup>
- Scaling with nuclear charge  $Z$ , for alkali atoms<sup>14</sup>

$$R \propto Z^3 \alpha^2$$

- Heavy atoms required. Typical values in practice:

$$Z > 50$$

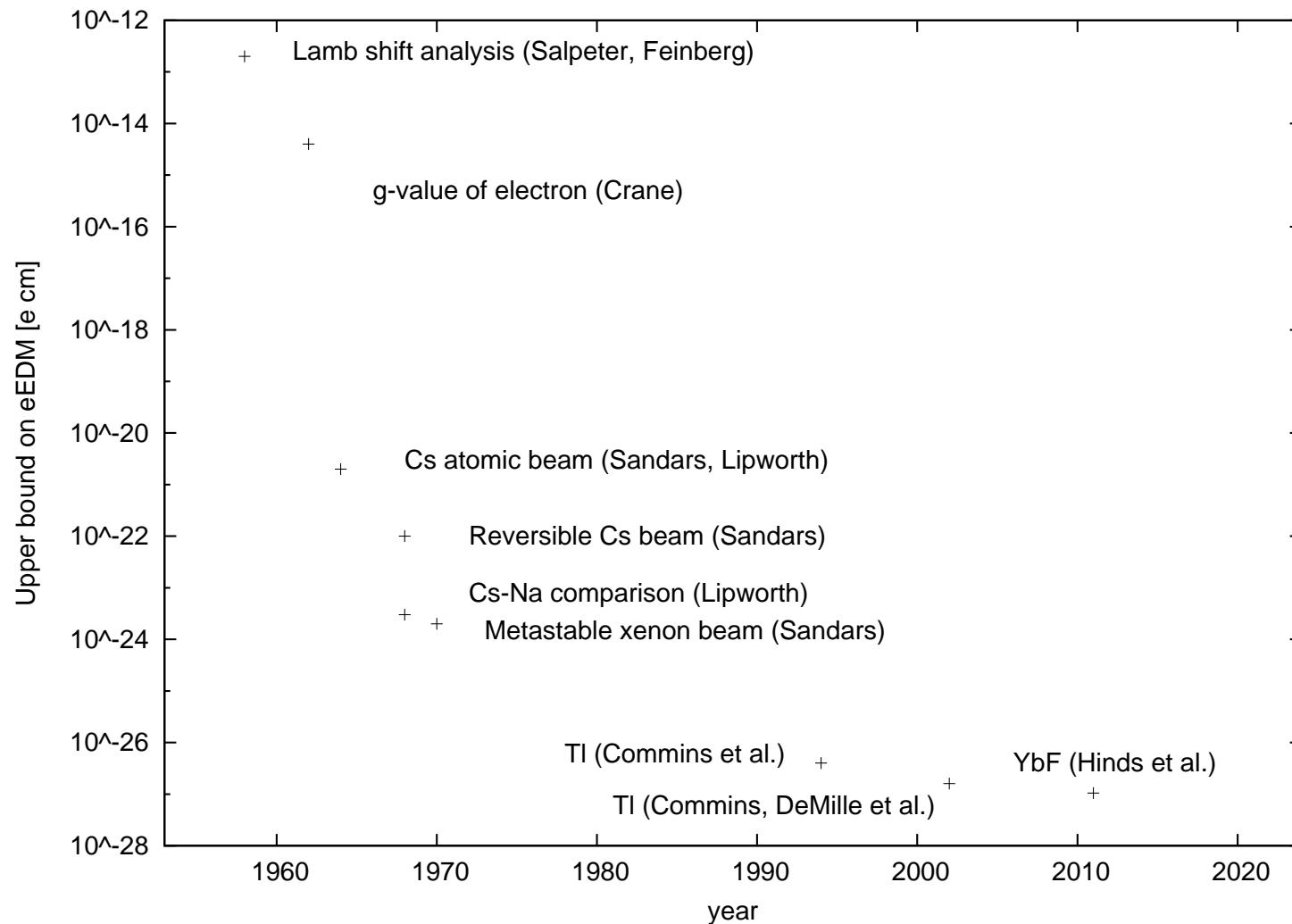
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<sup>12</sup>L.I. Schiff, *Phys Rev* **132** (1963) 2194

<sup>13</sup>E.D. Commins, J.D. Jackson, D.P. DeMille, *Am J Phys* **75** (2007) 532

<sup>14</sup>P.G.H. Sandars, *Phys Lett* **14** (1965) 194

# Historical Development of eEDM Upper Bound<sup>15</sup>



<sup>15</sup>Sandars (1975), Commins, DeMille (2008)

# The eEDM in a molecular framework

## Perturbative EDM operator

$\mathcal{P}$ - and  $\mathcal{T}$ -odd eEDM Hamiltonian<sup>16</sup>:

$$\hat{H}_{\text{EDM}} = -\frac{d_e}{4} \gamma^0 \gamma^5 (\gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu) F_{\mu\nu}$$

which comprises an electric and a “motional” part

$$\hat{H}_{\text{EDM}} = -d_e \gamma^0 [\Sigma \cdot \mathbf{E} + i \boldsymbol{\alpha} \cdot \mathbf{B}]$$

Magnetic contribution does not enter to leading order<sup>17</sup>

Electric field contributions

$$\mathbf{E} = \mathbf{E}_{\text{int}} + \mathbf{E}_{\text{ext}}$$

with an internal nuclear and electronic contribution

$$\mathbf{E}_{\text{int}}(i) = \sum_{A=1}^N \frac{Ze (\vec{r}_i - \vec{r}_A)}{||\vec{r}_i - \vec{r}_A||^3} - \sum_{j=1}^n \frac{e (\vec{r}_i - \vec{r}_j)}{||\vec{r}_i - \vec{r}_j||^3}$$

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<sup>16</sup>E. Salpeter, *Phys Rev* **112** (1958) 1642

<sup>17</sup>E. Lindroth, E. Lynn, P.G.H. Sandars, *J Phys B: At Mol Opt Phys* **22** (1989) 559

# The eEDM in a molecular framework

## Effective EDM many-body operator

Theoretical framework is relativistic quantum mechanics, no QED contributions

Exact reformulation of interaction constant for a single-particle expectation value<sup>18</sup>

$$\langle -d_e \gamma^0 \Sigma \cdot \mathbf{E} \rangle_{\psi^{(0)}} = \frac{2icd_e}{e\hbar} \langle \gamma^0 \gamma^5 \vec{p}^2 \rangle_{\psi^{(0)}}$$

Approximate effective expectation value in many-body system

$$-d_e \left\langle \sum_{j=1}^n \gamma^0(j) \Sigma(j) \cdot \mathbf{E}(j) \right\rangle_{\psi^{(0)}} \approx \frac{2icd_e}{e\hbar} \left\langle \sum_{j=1}^n \gamma^0(j) \gamma^5(j) \vec{p}(j)^2 \right\rangle_{\psi^{(0)}}$$

$\psi^{(0)}$  here is the atomic/molecular electronic wavefunction.

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<sup>18</sup>E. Commins, *Adv At Mol Opt Phys* **40** (1999) 1

# Correlated Wavefunction Theory for E<sub>eff</sub>

- Dirac-Coulomb Hamiltonian operator

$$\hat{H}^{DC} = \sum_A \sum_i [c(\vec{\alpha} \cdot \vec{p})_i + \beta_i m_0 c^2 + V_{iA}] + \sum_{i,j > i} \frac{1}{r_{ij}} \mathbb{1}_4 + \sum_{A,B > A} V_{AB}$$

- All-electron Dirac-Coulomb Hartree-Fock (DCHF) calculation  
set of time-reversal paired 4-spinors  $\hat{K}\varphi_i = \varphi_{\bar{i}}$  and  $\hat{K}\varphi_{\bar{i}} = -\varphi_i$
- Expansion and variation<sup>19</sup> in  $n$ -electron sector of Fock space

$$|\psi_k\rangle = \sum_{I=1}^{\dim \mathcal{F}^t(M,n)} c_{kI} |(\mathcal{S}\bar{\mathcal{T}})_I\rangle$$

Expectation values over relativistic Configuration Interaction wavefunctions<sup>20</sup>

$$\langle \hat{H}_{EDM} \rangle_{\psi_k^{(0)}} = \sum_{I,J=1}^{\dim \mathcal{F}^t(M,n)} c_{kI}^* c_{kJ} \left\langle (\mathcal{S}\bar{\mathcal{T}})_I \right| \frac{2icd_e}{e\hbar} \sum_{j=1}^n \gamma^0(j) \gamma^5(j) \vec{p}(j)^2 \left| (\mathcal{S}\bar{\mathcal{T}})_J \right\rangle$$

<sup>19</sup>S Knecht, H J Aa Jensen, TF, *J Chem Phys* **132** (2010) 014108

<sup>20</sup>TF and M K Nayak, *Phys Rev A* **88** (2013) 032514

# Search for the Electron EDM

## Why molecules?

Be an atom in a parity eigenstate  $\hat{\mathcal{P}} |\psi_p\rangle = \prod_{i=1}^n \hat{p}(i) \hat{\mathcal{A}} |\varphi_a(1) \cdot \dots \cdot \varphi_m(n)\rangle$ .

Then

$$\begin{aligned}\langle \psi_p | \hat{H}_{\text{EDM}} | \psi_p \rangle &= \langle \psi_p | \hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} \hat{H}_{\text{EDM}} \hat{\mathcal{P}}^\dagger \hat{\mathcal{P}} | \psi_p \rangle = -p^2 \langle \psi_p | \hat{H}_{\text{EDM}} | \psi_p \rangle \\ &= - \langle \psi_p | \hat{H}_{\text{EDM}} | \psi_p \rangle = 0\end{aligned}$$

Parity eigenstates need to be mixed (polarization).

1. A perturbing laboratory **E** field is required to mix parity eigenstates.  
TI experiment<sup>21</sup>  $E_{\text{eff}} \approx 0.05 \left[ \frac{\text{GV}}{\text{cm}} \right]$
2. Molecular fields:  
 $\text{YbF}^{22}$ :  $E_{\text{eff}} \approx 26 \left[ \frac{\text{GV}}{\text{cm}} \right]$ ,  $\text{HgF}^{23}$ :  $E_{\text{eff}} \approx 100 \left[ \frac{\text{GV}}{\text{cm}} \right]$ ,

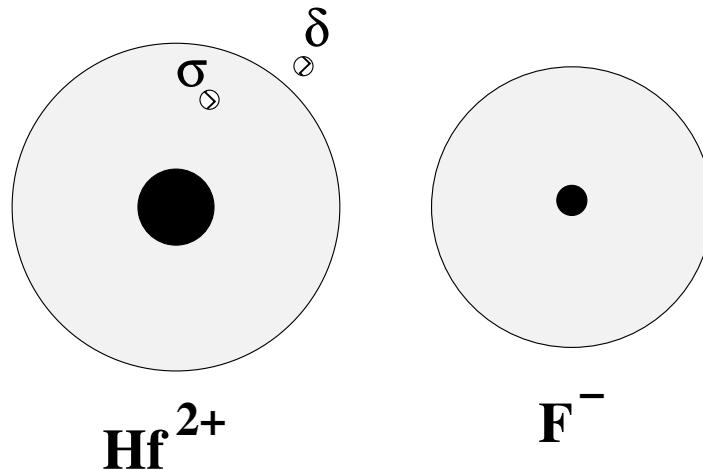
<sup>21</sup>V.V. Flambaum, *Sov J Nucl Phys* **24** (1976) 199

<sup>22</sup>D.M. Kara, I.J. Smallman, J.J. Hudson, B.E. Sauer, M.R. Tarbutt, E.A. Hinds, *New J Phys* **14** (2012) 103051

<sup>23</sup>Dmitriev et al., *Phys Lett* **167A** (1992) 280

# The eEDM in a molecular framework

$^3\Delta$  molecules<sup>24</sup>



- One heavy nucleus (relativistic effect)
- One “science” electron ( $\sigma^1$ ), one “spectroscopy” electron ( $\delta^1$ )
- Large  $E_{\text{eff}}$  for  $\sigma^1$  electron

- Deeply bound molecule (fluorides)
- Small  $\Lambda$  ( $\Omega$ )-doublet splitting<sup>25</sup> (optimal polarization)
- Large rotational constant (one heavy, one light atom)
- $\Omega = 1$  component preferred (small magnetic moment)  
⇒ Low-lying  $^3\Delta_1$  as “science” state

<sup>24</sup>E. Meyer, J. Bohn, D.A. Deskevich, *Phys Rev A* **73** (2006) 062108

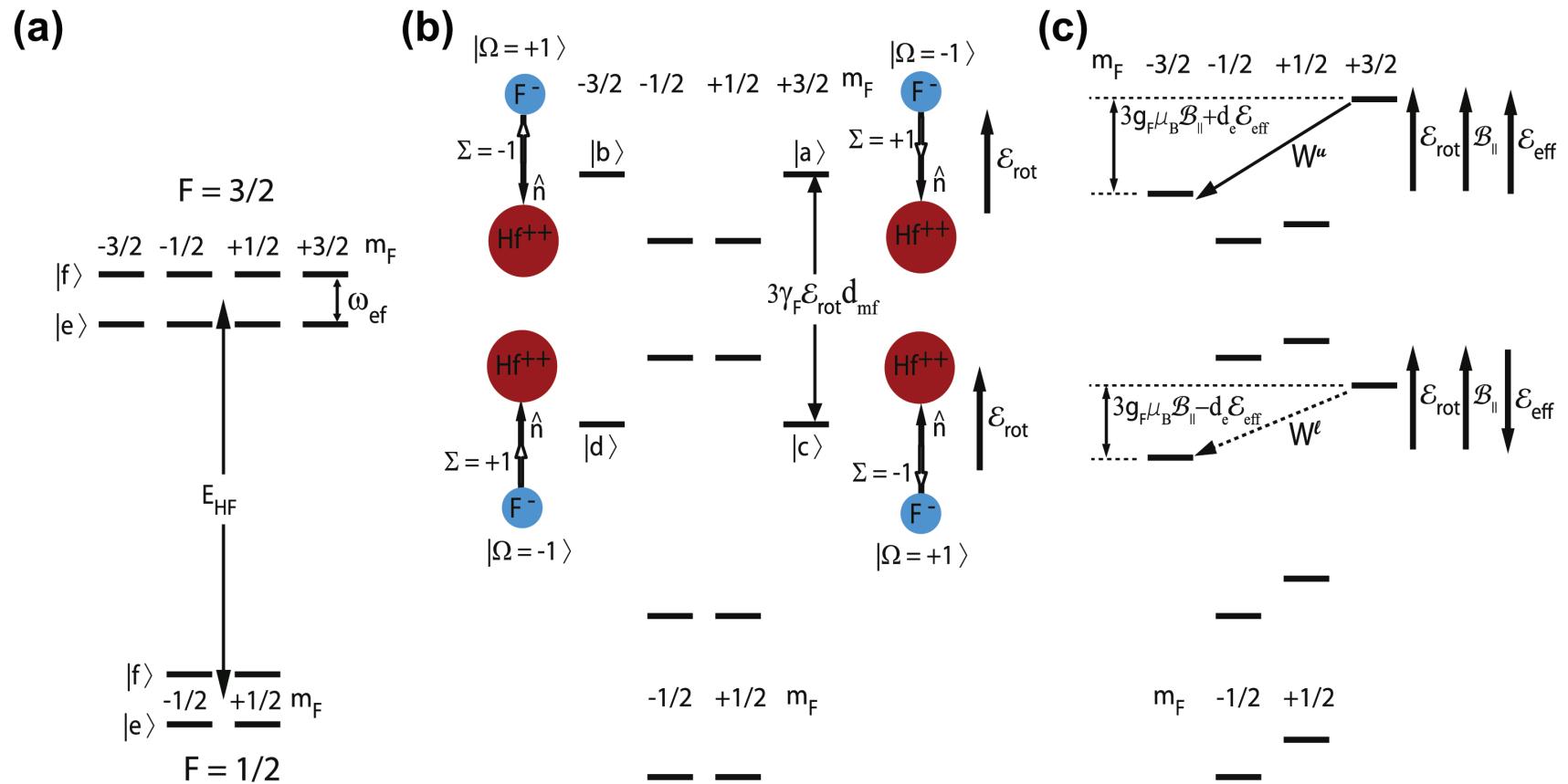
<sup>25</sup>TF, C.M. Marian, *J Mol Spectrosc* **178** (1996) 1

$\text{HfF}^+ / \text{ThF}^+$

JILA, Boulder, Colorado (Cornell group)

# The eEDM in a molecular framework

## A Proposed Measurement<sup>26</sup> on HfF<sup>+</sup>

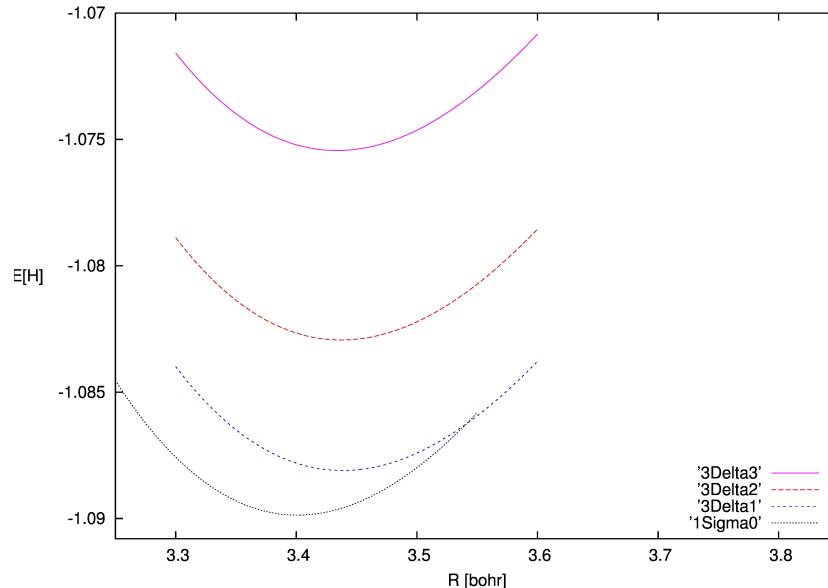


$$W^u(B) - W^u(-B) = 2d_e E_{\text{eff}}$$

<sup>26</sup>A.E. Leanhardt, J.L. Bohn, H. Loh, P. Maletinsky, E.R. Meyer, L.C. Sinclair, R.P. Stutz, E.A. Cornell, *J Mol Spectrosc* **270** (2011) 1

# HfF<sup>+</sup> electronic states and spectroscopic constants

$\Omega = 3$  (Hf<sup>2+</sup>6s<sup>1</sup>5d<sup>1</sup>)  
 $\Omega = 2$  (Hf<sup>2+</sup>6s<sup>1</sup>5d<sup>1</sup>)  
 $\Omega = 1$  (Hf<sup>2+</sup>6s<sup>1</sup>5d<sup>1</sup>)  
 $\Omega = 0$  (Hf<sup>2+</sup>6s<sup>2</sup>)



Model	R <sub>e</sub> [a.u.]				ω <sub>e</sub> [cm <sup>-1</sup> ]			
	Ω = 0	Ω = 1	Ω = 2	Ω = 3	Ω = 0	Ω = 1	Ω = 2	Ω = 3
CAS-CI(10)	3.400	3.436	3.434	3.431	796	774	775	778
MR-CISD(10)	3.506	3.558	3.557	3.552	656	643	643	644
MR-CISD+T(10)	3.510	3.560			654	643		
MR-CISD(20)	3.401	3.438	3.437	3.434	800	768	769	772
Experiment <sup>27</sup>					790.76	760.9		
Experiment <sup>28</sup>	3.374	3.407			791.2	761.3	762.3	761.5

<sup>27</sup>K. Cossel et al., *Chem. Phys. Lett.* **546** (2012) 1

<sup>28</sup>B.B. Barker, I.O. Antonov, V.E. Bondybey, M.C. Heaven, *J Chem Phys* **134** (2011) 201102

# HfF<sup>+</sup> and ThF<sup>+</sup>: $E_{\text{eff}}$ in the $\Omega = 1$ science state<sup>29</sup>

HfF <sup>+</sup>		ThF <sup>+</sup>	
Model	$E_{\text{eff}} \left[ \frac{\text{GV}}{\text{cm}} \right]$	Model	$E_{\text{eff}} \left[ \frac{\text{GV}}{\text{cm}} \right]$
CAS-CI(10)	24.1		
MR-CISD(10)	22.4		
MR-CISD(20)	23.3	MR <sub>3</sub> -CISD(18)	47.5
MR-CISD+T(20)	23.7	MR <sub>6</sub> -CISD(18)	36.2
MR-CISD(34)	22.9	MR <sub>10</sub> -CISD(18)	35.2
MR-CISD(34)+T	23.3	MR <sub>3</sub> -CISDT(18)	35.4
Estimate, Meyer et al. <sup>30</sup>	$\approx 30$	Meyer et al.	$\approx 90$
20 e <sup>-</sup> corr., Titov et al. <sup>31</sup>	24.2	36 e <sup>-</sup> corr., Titov et al.	$\approx 45$

(HfF<sup>+</sup>)

Similar results with various methods  
System currently under exp. study

(ThF<sup>+</sup>)

Different results with various methods  
Meyer's model inaccurate  
Titov's sr-CCSD(T) underestimates *s-p* mixing

<sup>29</sup> TF and M.K. Nayak, *Phys Rev A* **88** (2013) 032514

M. Denis, M.K. Nayak, TF, et al., *New J Phys* (2014) *in preparation*

<sup>30</sup> A.N. Petrov, N.S. Mosyagin, T.A. Isaev, A.V. Titov, *Phys Rev A* **76** (2007) 030501(R)

<sup>31</sup> E.R. Meyer, J.L. Bohn, *Phys Rev A* **78** (2008) 010502(R)

# ThO

ACME Collaboration, Yale/Harvard, (DeMille/Doyle/Gabrielse groups)

# Most Recent Measurement: ThO Molecule

## ACME Collaboration, Harvard/Yale



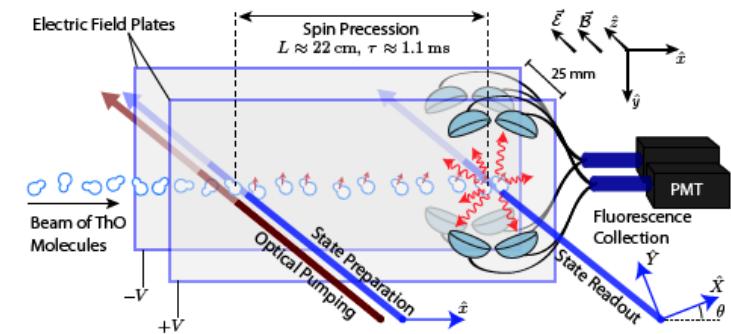
## Order of Magnitude Smaller Limit on the Electric Dipole Moment of the Electron

The ACME Collaboration\*: J. Baron<sup>1</sup>, W. C. Campbell<sup>2</sup>, D. DeMille<sup>3</sup>, J. M. Doyle<sup>1</sup>, G. Gabrielse<sup>1</sup>, Y. V. Gurevich<sup>1,\*,\*</sup>, P. W. Hess<sup>1</sup>, N. R. Hutzler<sup>1</sup>, E. Kirilov<sup>3,#</sup>, I. Kozyrev<sup>3,†</sup>, B. R. O'Leary<sup>3</sup>, C. D. Panda<sup>1</sup>, M. F. Parsons<sup>1</sup>, E. S. Petrik<sup>1</sup>, B. Spaun<sup>1</sup>, A. C. Vutha<sup>4</sup>, and A. D. West<sup>3</sup>

The Standard Model (SM) of particle physics fails to explain dark matter and why matter survived annihilation with antimatter following the Big Bang. Extensions to the SM, such as weak-scale Supersymmetry, may explain one or both of these phenomena by positing the existence of new particles and interactions that are asymmetric under time-reversal (T). These theories nearly always predict a small, yet potentially measurable ( $10^{-27}$ - $10^{-30}$  e cm) electron electric dipole moment (EDM,  $d_e$ ), which is an asymmetric charge distribution along the spin ( $\vec{S}$ ). The EDM is also asymmetric under T. Using the polar molecule thorium monoxide (ThO), we measure  $d_e = (-2.1 \pm 3.7_{\text{stat}} \pm 2.5_{\text{syst}}) \times 10^{-29}$  e cm. This corresponds to an upper limit of  $|d_e| < 8.7 \times 10^{-29}$  e cm with 90 percent confidence, an order of magnitude improvement in sensitivity compared to the previous best limits. Our result constrains T-violating physics at the TeV energy scale.

The exceptionally high internal effective electric field ( $\mathcal{E}_{\text{eff}}$ ) of heavy neutral atoms and molecules can be used to precisely probe

is prepared using optical pumping and state preparation lasers. Parallel electric ( $\vec{\mathcal{E}}$ ) and magnetic ( $\vec{\mathcal{B}}$ ) fields exert torques on the electric and magnetic dipole moments, causing the spin vector to precess in the  $xy$  plane. The precession angle is measured with a readout laser and fluorescence detection. A change in this angle as  $\vec{\mathcal{E}}_{\text{eff}}$  is reversed is proportional to  $d_e$ .



# Electron Electric Dipole Moment and Hyperfine Interaction Constants for ThO

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(Dated: June 10, 2014)

A recently implemented relativistic four-component configuration interaction approach to study  $\mathcal{P}$ - and  $\mathcal{T}$ -odd interaction constants in atoms and molecules is employed to determine the electron electric dipole moment effective electric field in the  $\Omega = 1$  first excited state of the ThO molecule. We obtain a value of  $E_{\text{eff}} = 75.2 \left[ \frac{\text{GV}}{\text{cm}} \right]$  with an estimated error bar of 3% and 10% smaller than a previously reported result [*J. Chem. Phys.*, 139:221103, 2013]. Using the same wavefunction model we obtain an excitation energy of  $T_v^{\Omega=1} = 5410 \left[ \text{cm}^{-1} \right]$ , in accord with the experimental value within 2%. In addition, we report the implementation of the magnetic hyperfine interaction constant  $A_{||}$  as an expectation value, resulting in  $A_{||} = -1339 \left[ \text{MHz} \right]$  for the  $\Omega = 1$  state in ThO. The smaller effective electric field increases the previously determined upper bound [*Science*, 343:269, 2014] on the electron electric dipole moment to  $|d_e| < 9.7 \times 10^{-29} e \text{ cm}$  and thus mildly mitigates constraints to possible extensions of the Standard Model of particle physics.

1401.2284v2

*J Mol Spectrosc* **300** (2014) 16

cm60, Düsseldorf, June 20, 2014

# The eEDM in ThO ( $\Omega = 1$ )

## Molecular Wavefunction for the “Science” State

	# of Kramers pairs	accumulated # of electrons min.    max.	
<i>Deleted</i>	(176)		
<i>Virtual</i>	183-K	36    36	$^3\Delta_1$ is the first molecular excited state
<i>Th: 6d<math>\sigma</math>, 7p, 8s Th: 7s, 6d<math>\delta</math></i>	K	36-m    36	$7s^16d\delta^1$ configuration considerably mixed in this state
<i>Th: 6s, 6p O: 2s, 2p</i>	8	34-n    34	
<i>Th: 5d</i>	5	18-p    18	CI expansion space
<i>Th: 5s, 5p</i>	4	8-q    8	$\leq 500.000.000$ terms
<i>Frozen core</i>	(31)		

# The eEDM in ThO ( $\Omega = 1$ )

## Basis Sets

Basis set/CI Model	$T_v$ [cm $^{-1}$ ]	$E_{\text{eff}}$ [GV/cm]	$A_{  }$ [MHz]
vDZ/MR <sub>3</sub> -CISD(18)	4535	80.8	-1283
vTZ/MR <sub>3</sub> -CISD(18)	3832	81.0	-1292
vQZ/MR <sub>3</sub> -CISD(18)	3643	80.7	-1298

Vertical excitation energy, effective electric field, and hyperfine constant at an internuclear distance of  $R = 3.477$  a<sub>0</sub> for  $\Omega = 1$  using basis sets with increasing cardinal number and the wavefunction model MR<sub>3</sub>-CISD(18)

Magnetic hyperfine interaction constant:

$$A_{||} = \frac{\mu_{Th}}{I\Omega} \left\langle \sum_{i=1}^n \left( \frac{\vec{\alpha}_i \times \vec{r}_i}{r_i^3} \right)_z \right\rangle_{\psi}$$

# The eEDM in ThO ( $\Omega = 1$ )

## Number of Correlated Electrons

CI Model	$T_v$ [cm $^{-1}$ ]	$E_{\text{eff}}$ [GV/cm]	$A_{  }$ [MHz]
MR-CISD(2)	5929	68.5	-1264
MR <sub>3</sub> -CISD(18)	3832	81.0	-1292
MR <sub>3</sub> -CISD(28)	3752	80.0	-1297
MR <sub>3</sub> -CISD(36) <sup>32</sup>	3742	80.8	-1287

Vertical excitation energy, effective electric field, and hyperfine constant at an internuclear distance of  $R = 3.477$  a<sub>0</sub> for  $\Omega = 1$  correlating only the atomic valence shells down to including core-valence and core-core correlation and using the vTZ basis sets

1401.2284v2

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<sup>32</sup>Due to extreme computational demand the virtual cutoff is 5 a.u. here.

# The eEDM in ThO ( $\Omega = 1$ )

## Active 4-Spinor Spaces

CI Model	$T_v$ [cm $^{-1}$ ]	$E_{\text{eff}}$ [GV/cm]	$A_{  }$ [MHz]
MR <sub>3</sub> -CISD(18)	3832	81.0	-1292
MR <sub>5</sub> -CISD(18)	4054	79.7	-1291
MR <sub>7</sub> -CISD(18)	4321	80.1	-1318
MR <sub>10</sub> -CISD(18)	5329	75.6	-1335
MR <sub>13</sub> -CISD(18)	<b>5437</b>	<b>75.2</b>	<b>-1339</b>
Exp. ( $T_e$ ) <sup>33</sup>	5317		

Vertical excitation energy, effective electric field, and hyperfine constant at an internuclear distance of  $R = 3.477$  a<sub>0</sub> for  $\Omega = 1$  using the vTZ basis set and varying active spinor spaces

1401.2284v2

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<sup>33</sup>J. Paulovič, T. Nakajima, K. Hirao, R. Lindh, and P.-Å. Malmqvist, *J. Chem. Phys.* **119** (2003) 798

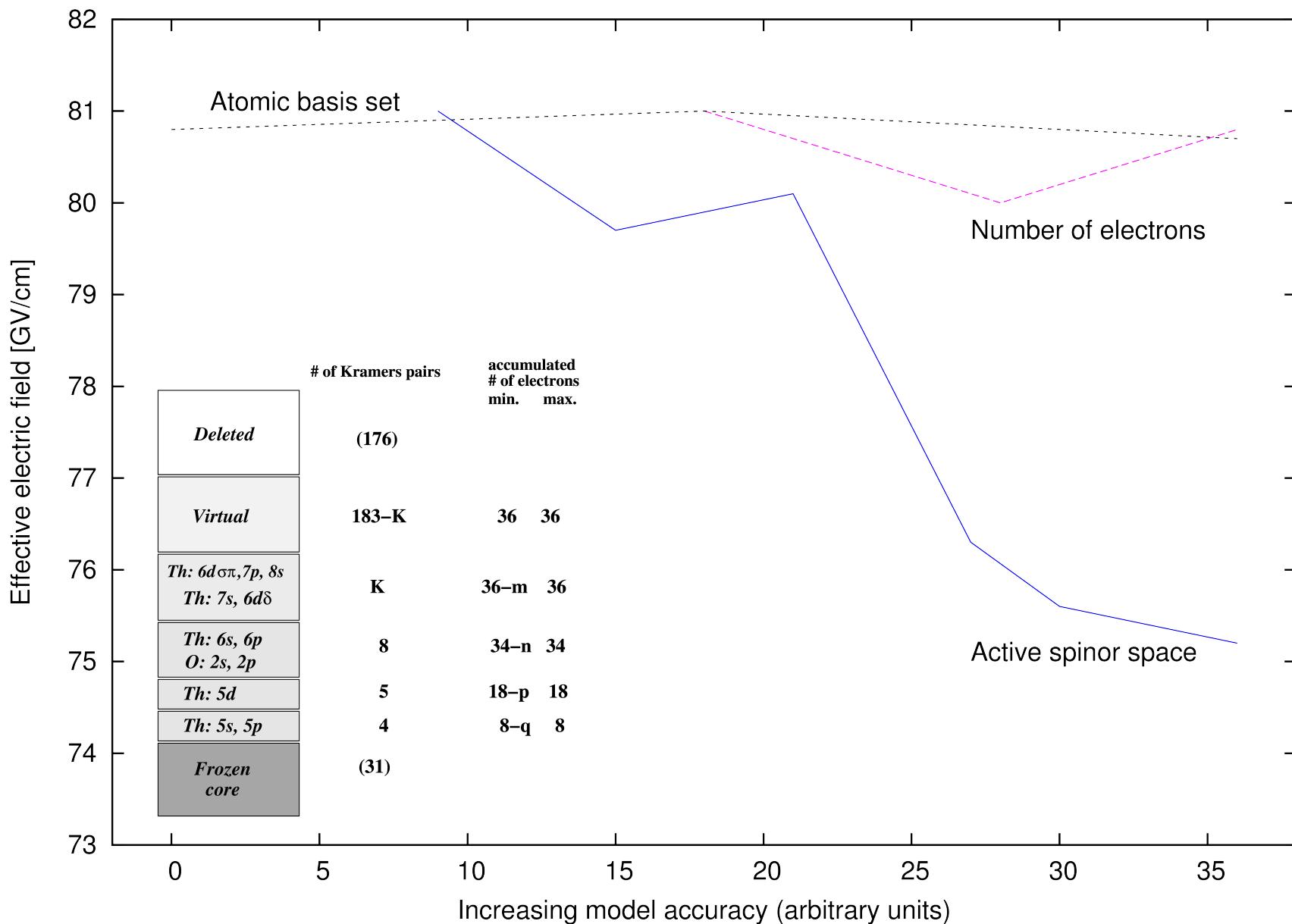
# The eEDM in ThO ( $\Omega = 1$ )

## Higher Excitations

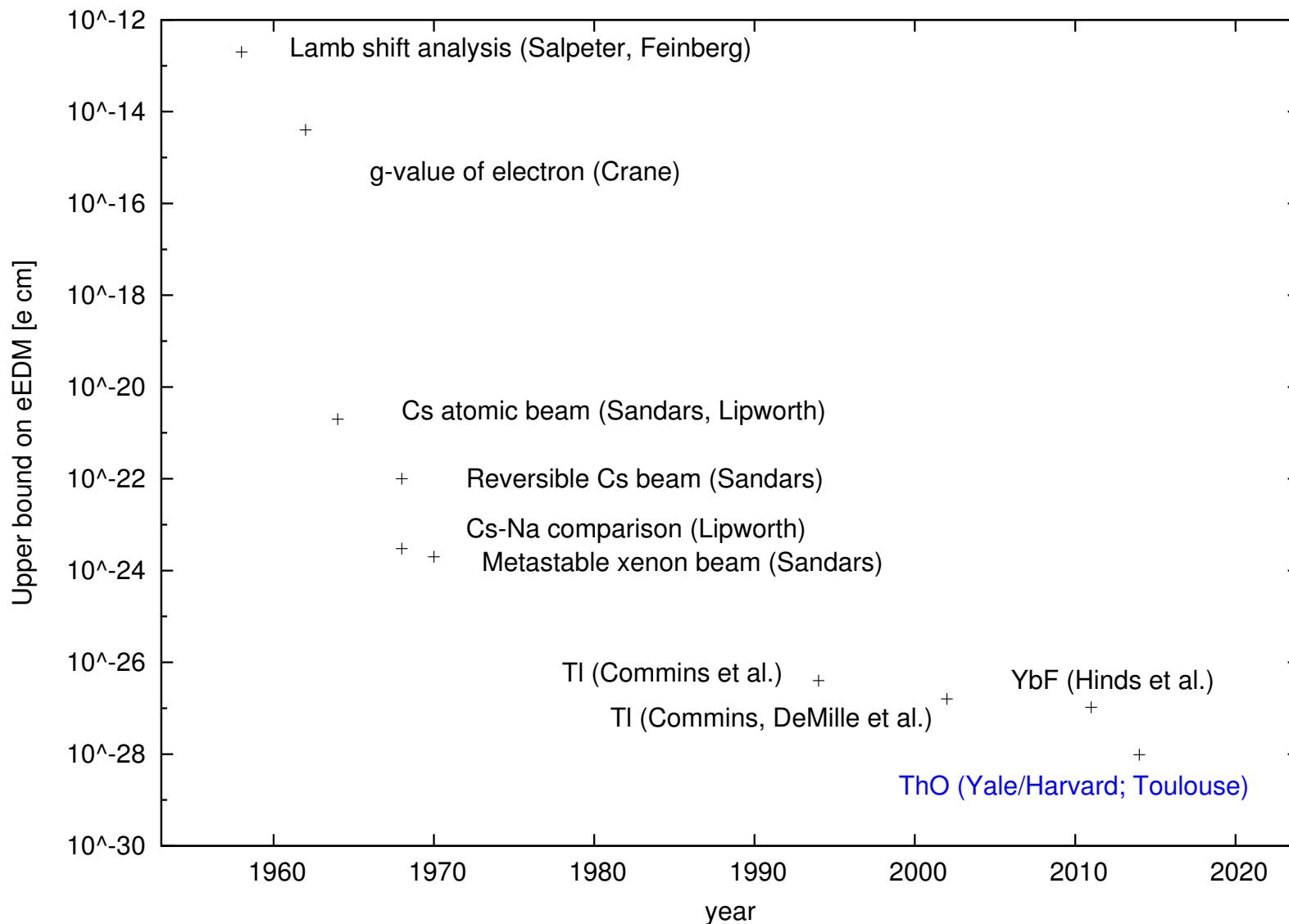
CI Model	$T_v$ [cm $^{-1}$ ]	$E_{\text{eff}}$ [GV/cm]	$A_{  }$ [MHz]
MR <sub>3</sub> -CISD(18)	4535	80.8	-1283
MR <sub>9</sub> -CISD(18)	5703	73.8	-1321
MR <sub>3</sub> -CISDT(18)	5166	74.5	-1340

Vertical excitation energy, effective electric field, and hyperfine constant at an internuclear distance of  $R = 3.477$  a<sub>0</sub> for  $\Omega = 1$  using the vDZ basis set and varying maximum excitation rank

# The eEDM in ThO ( $\Omega = 1$ )

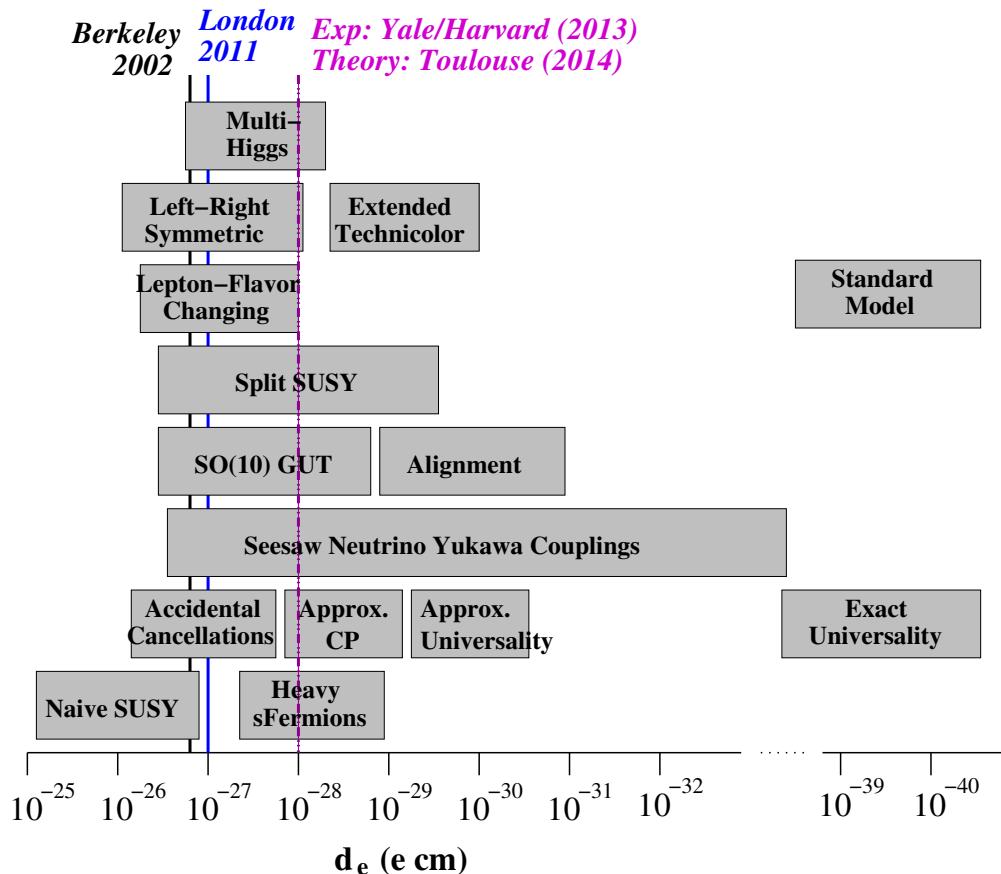


# Historical Development of eEDM Upper Bound<sup>34</sup>



<sup>34</sup>Sandars (1975), Commins, DeMille (2008)

# eEDM Constraint on Beyond-Standard-Model Theories<sup>35</sup>



Model	$ d_e  [e \cdot cm]$
Standard model	$< 10^{-38}$
Left-right symmetric	$10^{-28} \dots 10^{-26}$
Lepton-flavor changing	$10^{-29} \dots 10^{-26}$
Multi-Higgs	$10^{-28} \dots 10^{-27}$
Supersymmetric	$\leq 10^{-25}$
Experimental limit (TI) <sup>36</sup>	$< 1.6 \cdot 10^{-27}$
Experimental limit (YbF) <sup>37</sup>	$< 10.5 \cdot 10^{-28}$
Experimental limit (ThO) <sup>38</sup>	$< 9.7 \cdot 10^{-29}$

<sup>35</sup>Courtesy: DeMille (2005), Huliyar (2009)

<sup>36</sup>B.C. Regan, E.D. Commins, C.J. Schmidt, D.P. DeMille, *Phys Rev Lett* **88** (2002) 071805/1

<sup>37</sup>J.J. Hudson, D.M. Kara, I.J. Smallman, B.E. Sauer, M.R. Tarbutt, E.A. Hinds, *Nature* **473** (2011) 493

<sup>38</sup>ACME Collaboration, *Science* **6168** (2014) 269, T. Fleig and M. K. Nayak, *J. Mol. Spectrosc.* **300** (2014) 16

# Outlook

Project EDMeDM.



- Hyperfine interaction constants for an experimentally known diatomic molecule comparison with our calculations ( $\text{WC}^{39}$ )
- Scalar-pseudoscalar  $\mathcal{P}$  and  $\mathcal{T}$  odd electron-nucleon interaction constant  $C_S$
- Development of approximately size-extensive approach to calculation of enhancement factors (Coupled Cluster theory)
- Study of other diatomic molecules (in particular  $\text{ThF}^+$  (JILA, Boulder),  $\text{WC}$  (Leanhardt, Ann Arbor))
- Nuclear Schiff moment electronic-structure study (diamagnetic systems)

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<sup>39</sup>J. Lee, J. Chen, L. V. Skripnikov, A. N. Petrov, A. V. Titov, N. S. Mosyagin, A. E. Leanhardt, *Phys Rev A* **87** (2013) 2013