

Prospective Candidates for EDM  
Experiments of New Type:  
Calculations of EDM Enhancement  
in  $\text{HI}^+$  and Liquid Xe.

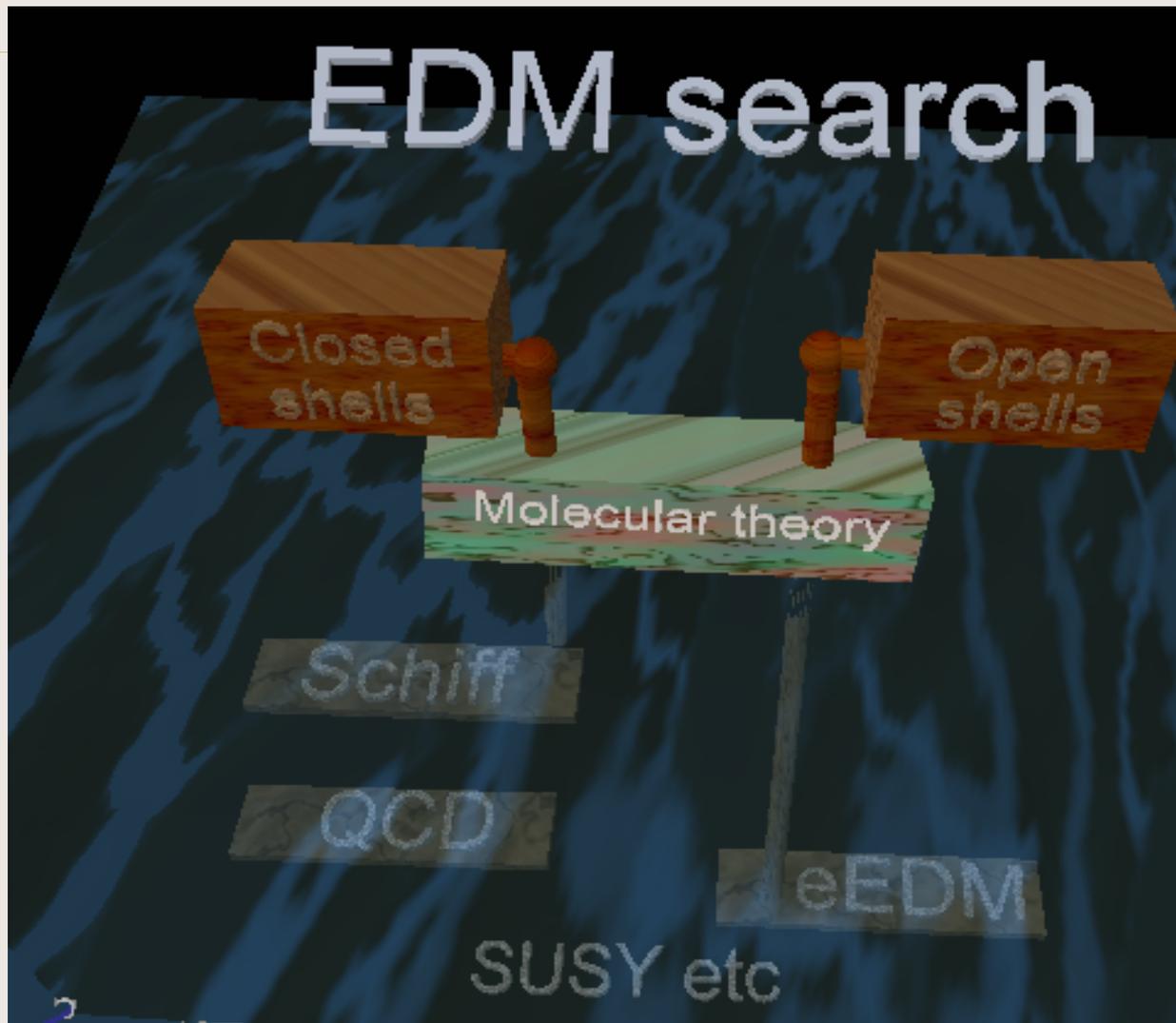
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# Search for “New Physics”



# Current Experiments on EDM Search

- **YbF** molecular beam experiment (*Imperial College, UK, group of E.Hinds*) 
- **PbO** optic cell experiment (*Yale University, USA, group of D.DeMille*) 
- **GdIG** garnet, solid state (L.R.Hunter, *Amherst, S.K.Lamoreaux, LANL*)

# Experiments of New Type

## Electron EDM

On diatomic hydride cations with ground state  $\Omega \geq 1$  ( $\Pi$ ,  $\Delta$ , ...- states)

## Nuclear Schiff Moment (Proton EDM)

- In liquids (Xe, Xe+polar diatomics)
- In solid state ( $\text{PbTiO}_3$ )

All the experimental objects present a challenge for molecular theory

# Challenge To Theory

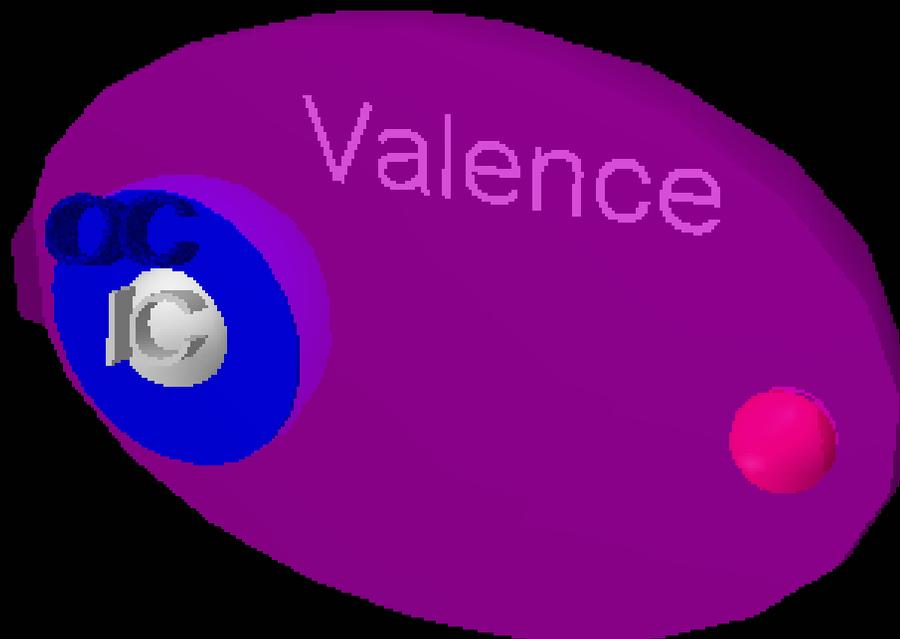
1. Ground  $\Delta$ -state means transition metal (or actinides) hydrides. Calculations of the electronic structure for transition metals (actinides) and their compounds is considered as non-trivial task in molecular theory (Nature **433(848)** 2005, U<sub>2</sub> molecule).
2. Liquid or solid state means accounting for large number of the electrons.

# Hydride Cations With $\Pi$ Ground State

Typical example is  $\text{HI}^+$  - ground state configuration is  $\sigma^2\pi_{1/2}^2\pi_{3/2}^1$ . Because unpaired electron is  $\pi_{3/2}$ , one cannot expect great enhancement of electron EDM. Unfortunately, there are some more reasons for EDM suppression in  $\text{HI}^+$ .

# Methods of Calculations

D i a t o m i c



# Methods of Calculations

- **GRECP/NOCR Method** (N.S. Mosyagin *et al*, Phys Rev A., **50**, 1994; A.V. Titov Int J. Quant. Chem, **57**, 1996)
- **Correlation Methods: RCC** (U.Kaldor, E.Eliav, A. Landau, Tel-Aviv, Israel ); **SODCI** (R.Buenker *et al*, Wuppertal, Germany )
- **Basis Sets** (N.S.Mosyagin *et al*, J. Phys.B, **33**, 2000; T.A. Isaev *et al*, J.Phys B, **33**, 2000)
- **Methods Development** (T.A. Isaev *et al*, J.Phys B, **33**, 2000; A.N. Petrov *et al*, Phys. Rev A. , **72** 2005)

# What Is Calculated

- $H_{P,T\text{-odd}} = W_d d_e (\mathbf{J} \cdot \mathbf{n})$ , where  $d_e = |\mathbf{d}_e|$ ,  $(\mathbf{J} \cdot \mathbf{n}) = \Omega$  - projection of the electron moment on molecular axis,  
 $W_d$  – characterizes electron EDM enhancement.
- The value of  $W_d |\Omega|$  can be considered as some effective electric field on electron,  
 $E_{\text{eff}} \equiv W_d |\Omega|$ . It is not zero only because of relativistic effects,

# On HI<sup>+</sup> Model

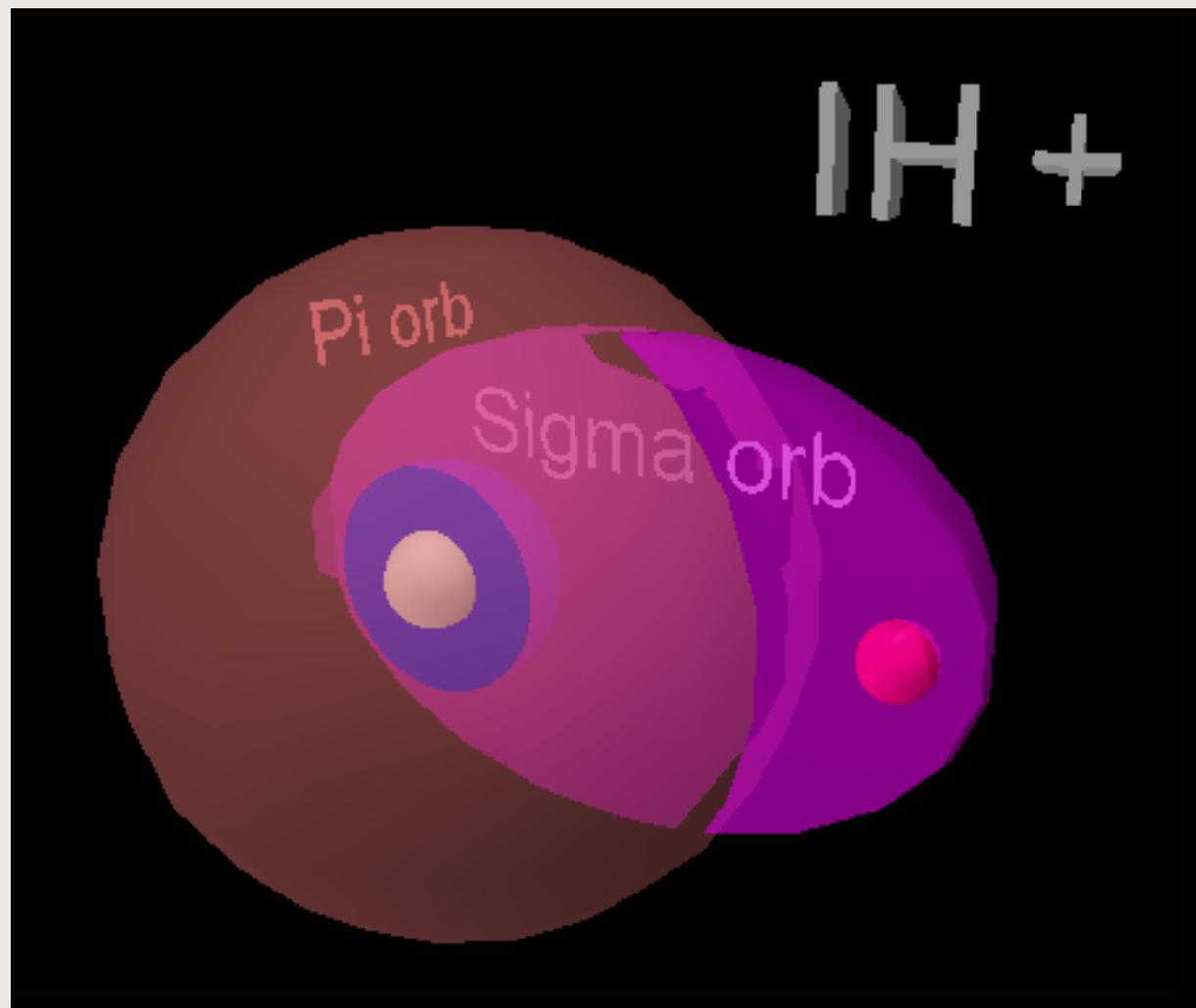
HI<sup>+</sup> ground state configuration in  $\lambda s$ -notation  
(nonrelativistic)  $\sigma^2\pi^3$

Highest **doubly** occupied  $\sigma$ -orbital is **bonding**  
and most “mixed”:

$$\sigma = 5p_0(\text{I}) + 1s(\text{H})$$

This is **not the highest by energy** from the  
occupied orbitals, **but gives 77%** of the  
molecular dipole moment

# On $\text{H}^+$ Model



# HI<sup>+</sup> Calculations

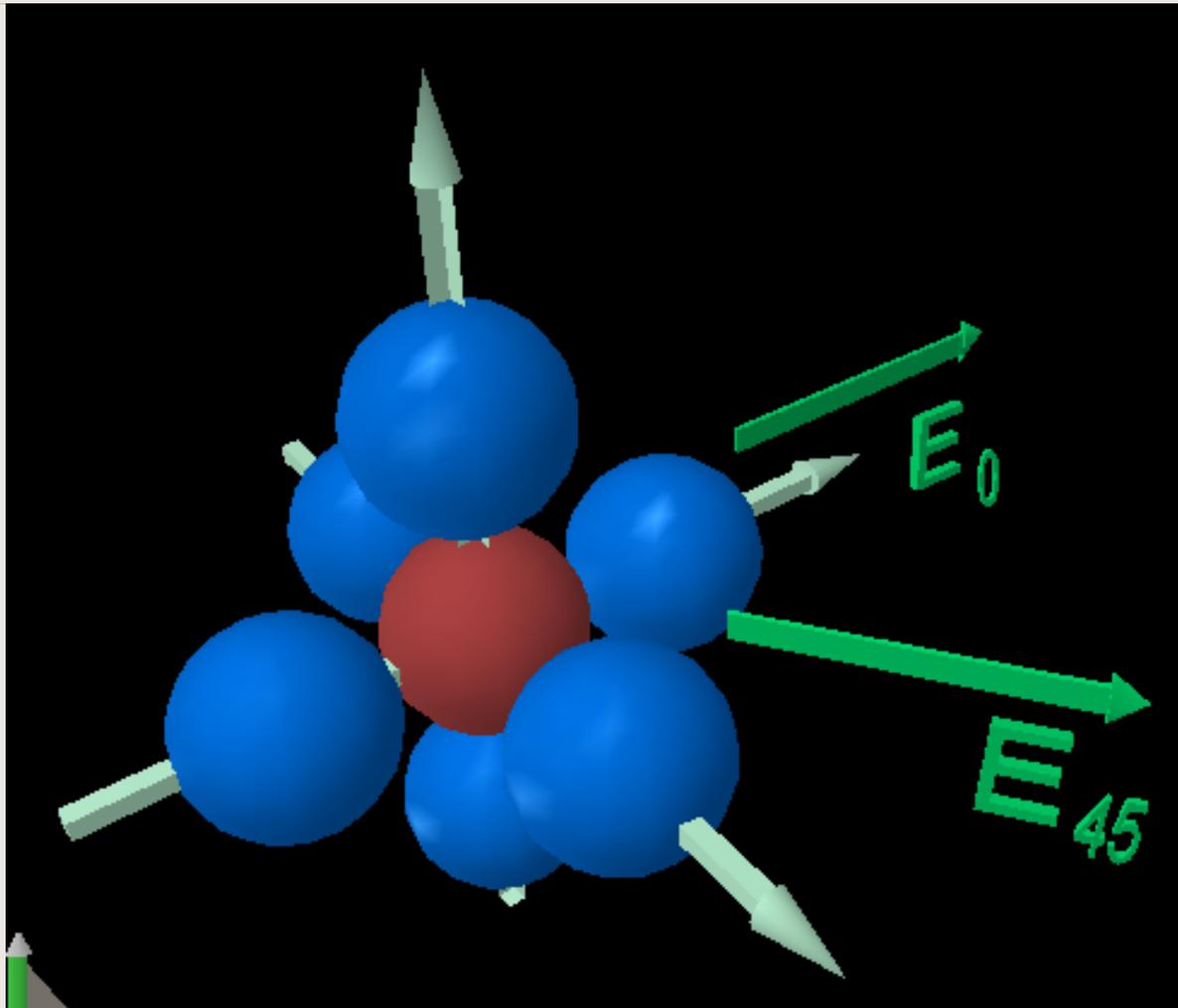
TABLE I: Calculated  $E_{\text{eff}}$  (in  $\times 10^{24}$  Hz/(e-cm)),  $A_{\parallel}$  (in MHz) and quadrupole interaction value  $eQq_0$  (in MHz) for the ground state  $X^2\Pi_{3/2}$  of  $\text{H}^{127}\text{I}^+$ . Experimental values for  $A_{\parallel}$  is 1021 MHz and for quadrupole coupling constant  $eQq_0$  is -712.6 MHz.

Method		$E_{\text{eff}}$	$A_{\parallel}$	$eQq_0$
work [Ravaine <i>et al.</i> ]	“ionic” approx. DHF	-0.09		
work [Ravaine <i>et al.</i> ]	“covalent” approx. CI	-0.49		
<b>AGRECP/SCF calculations</b>				
restricted SCF	<i>7 electrons</i>	0.008	949	-647
<b>GRECP/RCC calculations</b>				
RCC-S	<i>7 electrons</i>	0.206	863	-719
RCC-S	<i>25 electrons</i>	0.226	906	-807
RCC-SD	<i>25 electrons</i>	0.345	962	-752
<b>GRECP/SODCI calculations</b>				
Thresh.(mHartree)	SAF number			
	<i>25 electrons</i>			
0.0003	12 678 133	0.336	968	-745

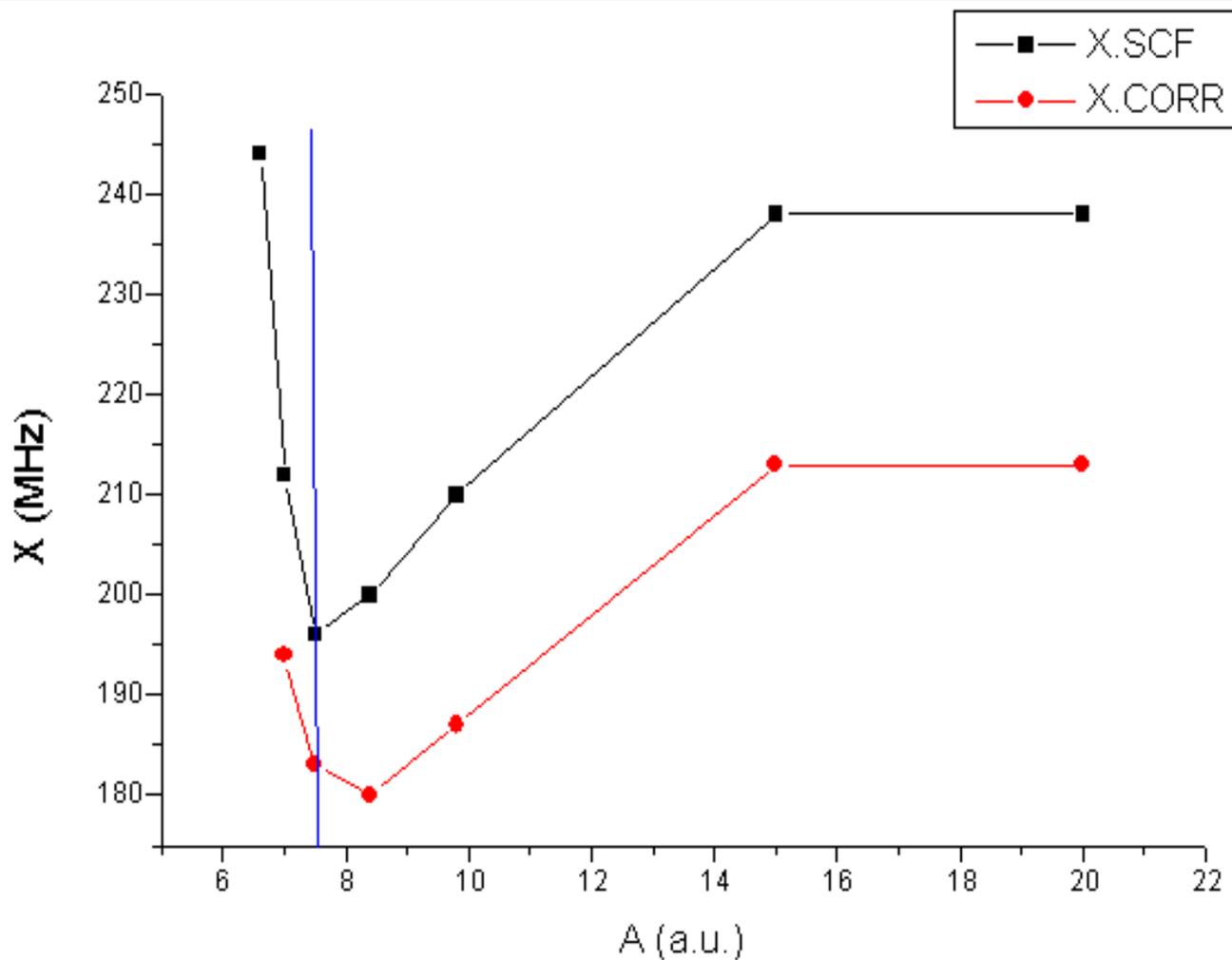
a(1) metastable state in PbO molecule

6.0

# Cluster Model of Liquid Xenon



# Cluster Model of Liquid Xenon



A spiral-bound notebook with a light beige, textured cover. The spiral binding is on the left side. The text "Thank You!" is centered on the cover in a black, serif font.

Thank You!