Search for electron EDM in molecular experiments: new objects and importance of precise calculations.

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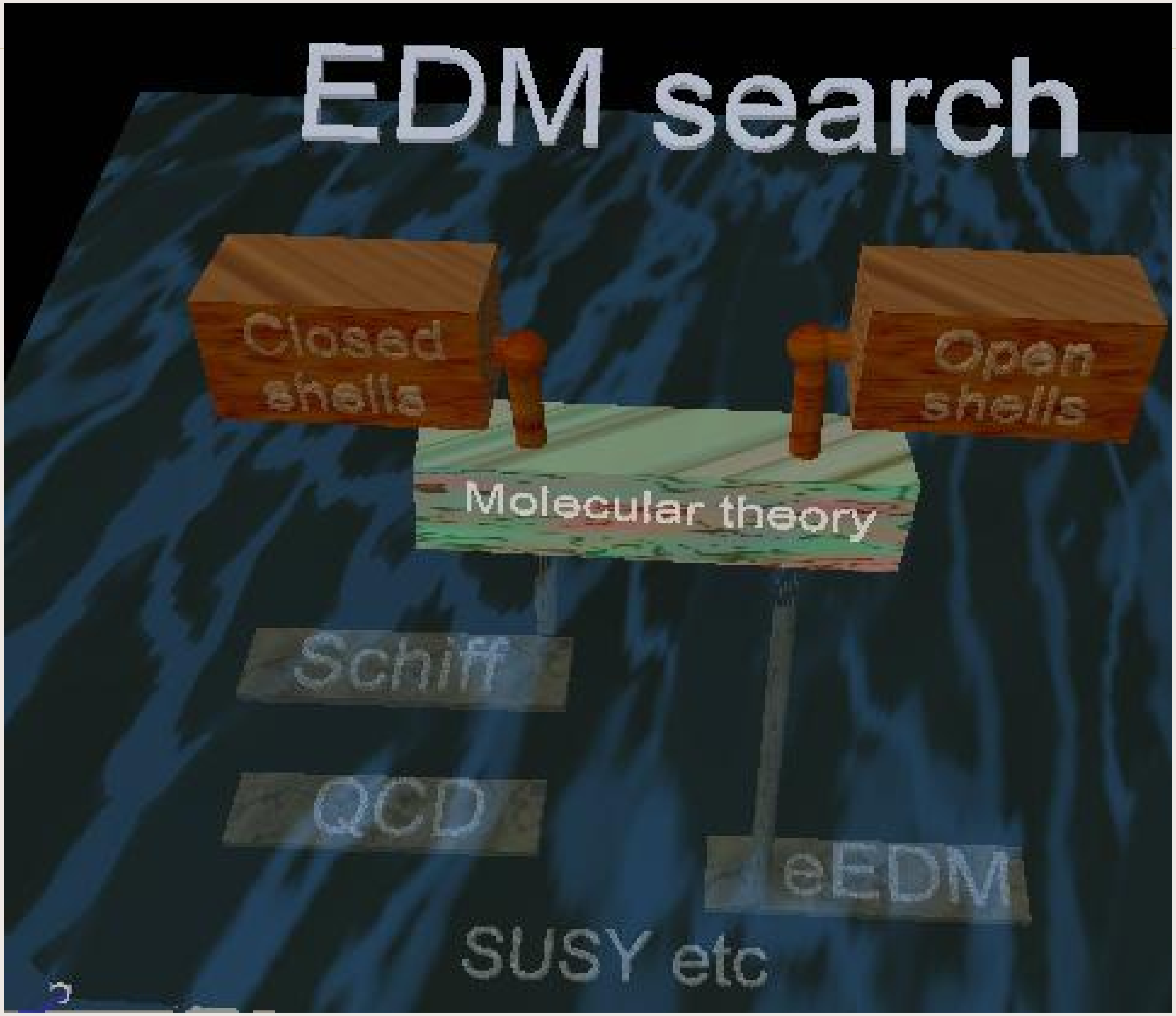
Search for “New Physics”



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.D[illegible]ille)
- 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 $\Omega \geq 1$ (Π, Δ, …- states)

Nuclear Schiff Moment (Proton EDM)

- In liquids (Xe, Xe+polar diatomics)
- In solid state ($PbTiO_3$)

All the experimental objects present a challenge for molecular theory

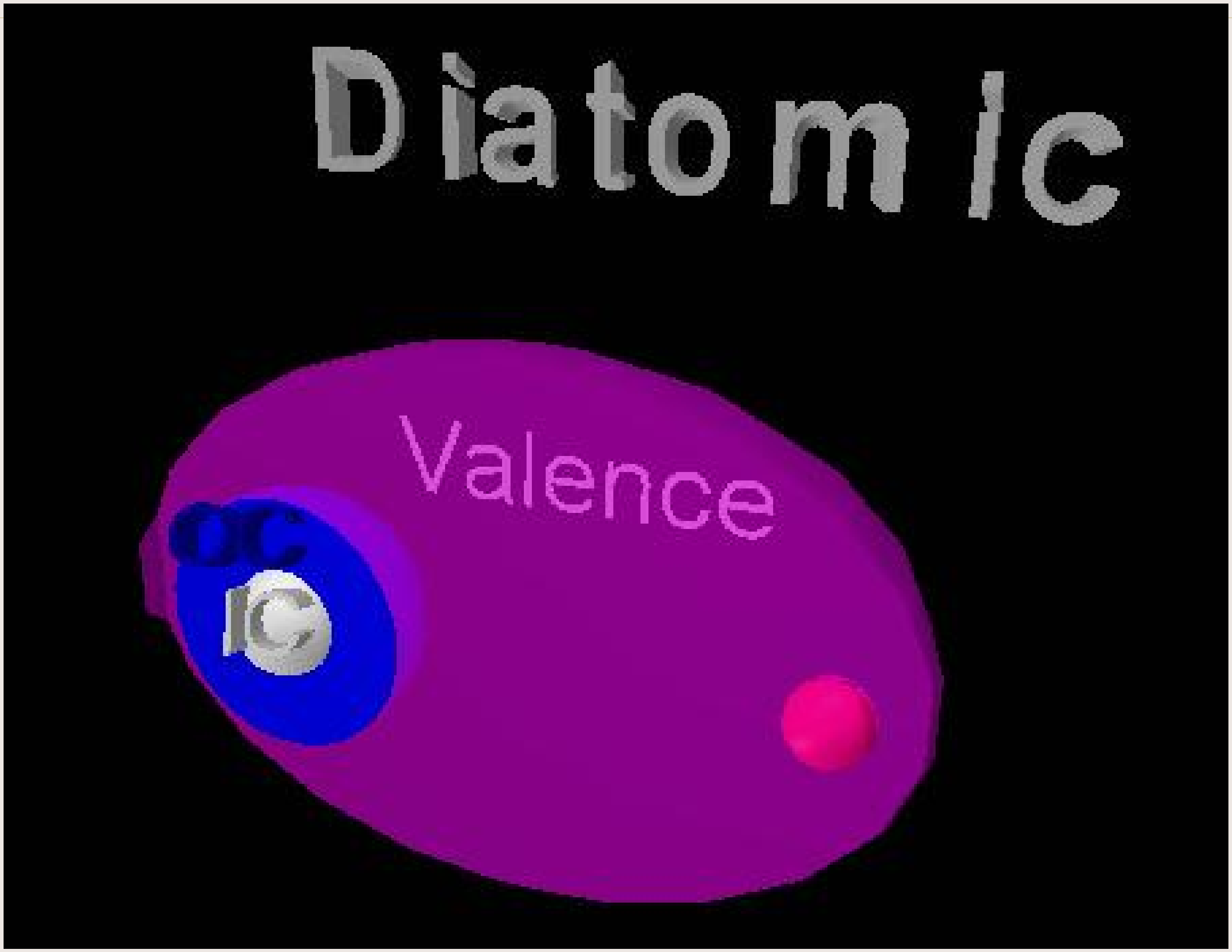
Challenge To Theory

1. Ground Δ-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_2 molecule).
2. Liquid or solid state means accounting for large number of the electrons.

Hydride Cations With Π Ground State

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

Methods of Calculations



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

- $H_{P,T\text{-}odd} = W_d\, d_e\, (\boldsymbol{J}\cdot \boldsymbol{n})$, where $d_e = |\,\mathbf{d_e}\,|$, $(\boldsymbol{J}\cdot \boldsymbol{n}) = \Omega$ - 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, $E_{eff} \equiv W_d\,|\Omega|$. It is not zero only because of relativistic effects,

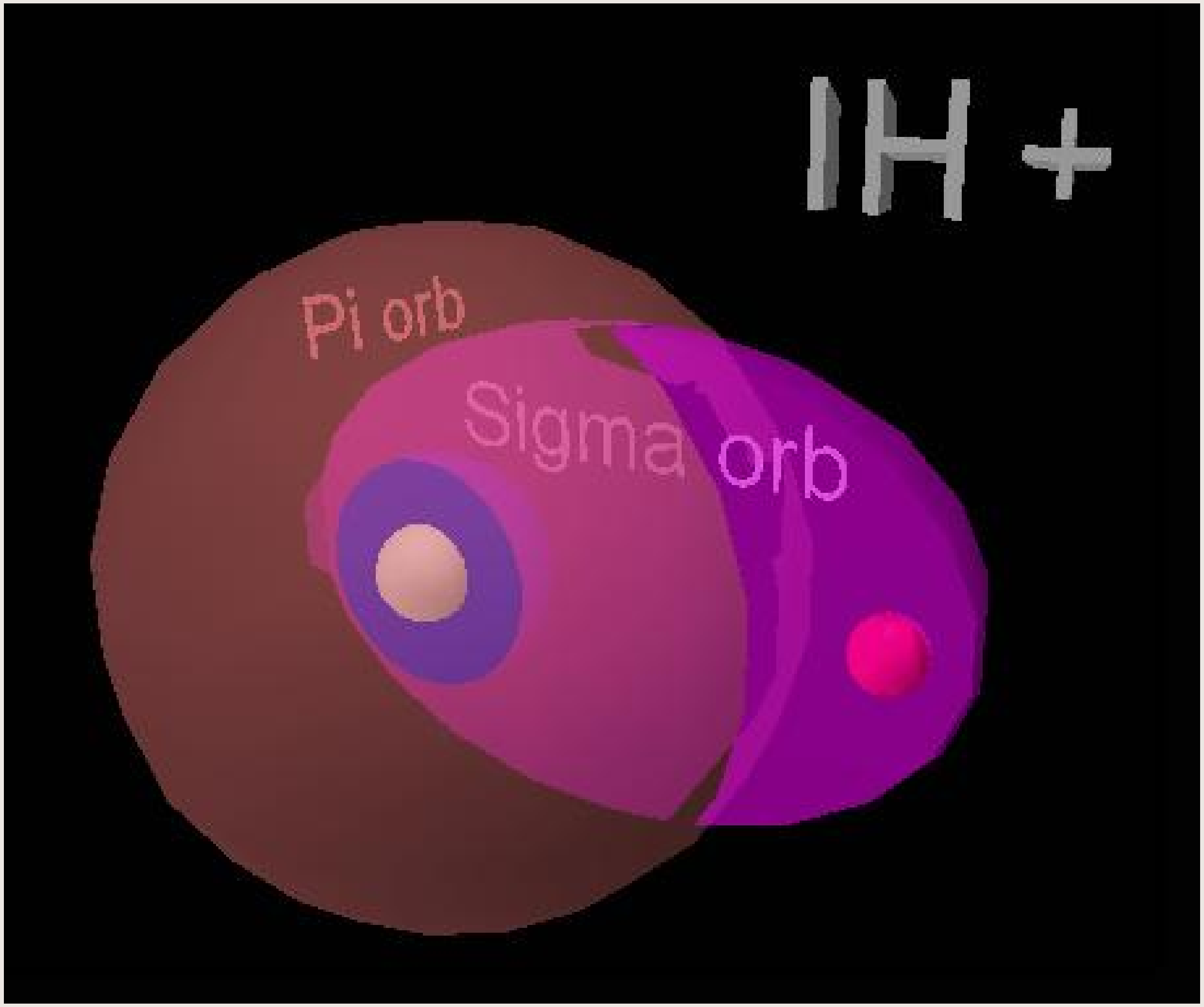
On HI^+ Model

HI^+ ground state configuration in λs-notation (nonrelativistic) s^2p^3

Highest doubly occupied σ-orbital is bonding and most "mixed":
$\sigma \sim 5p_0(I) + 1s(H)$

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

On HI^+ Model

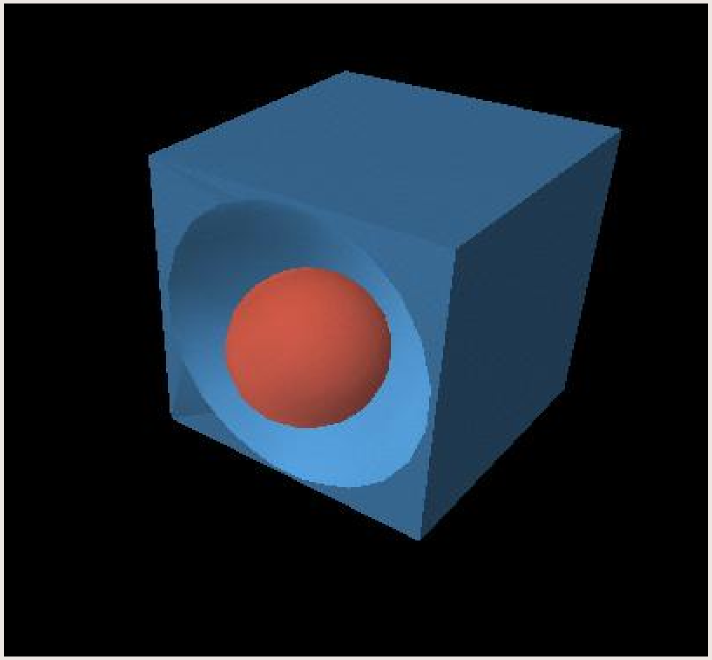


HI$^+$ Calculations

TABLE I: Calculated $E_{\rm eff}$ (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 $H^{127}I^+$. Experimental values for $A_\parallel$ is 1021 MHz and for quadrupole coupling constant eQq_0 is -712.6 MHz.

Method		$E_{\rm eff}$	$A_\parallel$	eQq_0
work [Ravaine *et al.*] "ionic" approx. DHF		-0.09		
work [Ravaine *et al.*] "covalent" approx. CI		-0.49		
AGRECP/SCF calculations				
resticted SCF	*7 electrons*	0.008	949	-647
GRECP/RCC calculations				
RCC-S	*7 electrons*	0.206	863	-719
RCC-S	*25 electrons*	0.226	906	-807
RCC-SD	*25 electrons*	0.345	962	-752
GRECP/SODCI calculations				
Thresh.(mHartree)	SAF number			
	25 electrons			
0.0003	12 678 133	0.336	968	-745
a(1) metastable state in PbO molecule				
		6.0		

Liquid Xenon
Cavity (cell) model



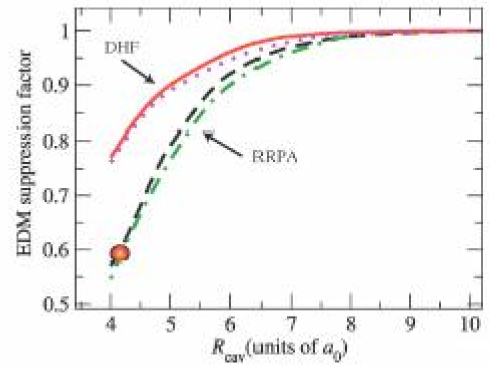
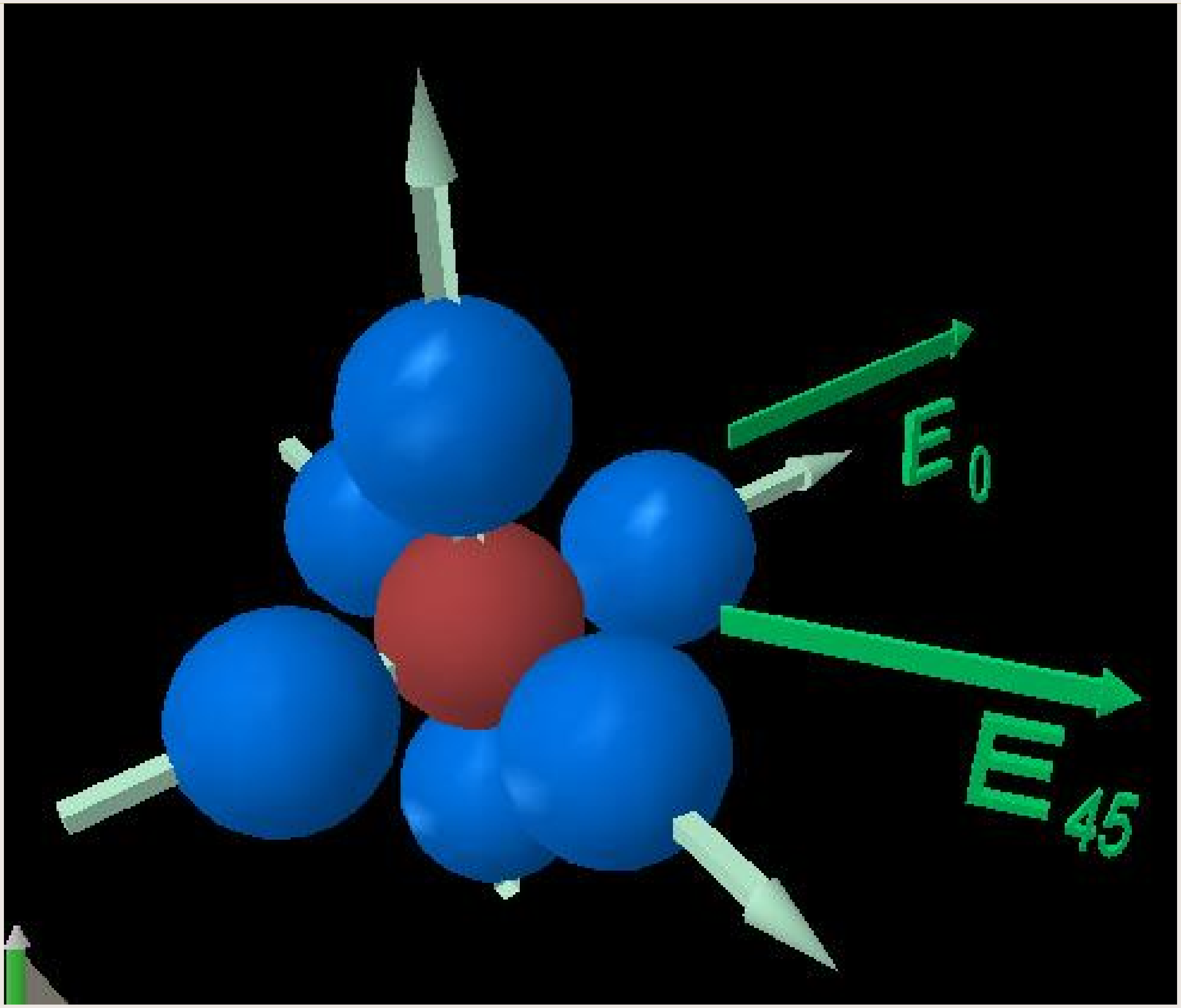
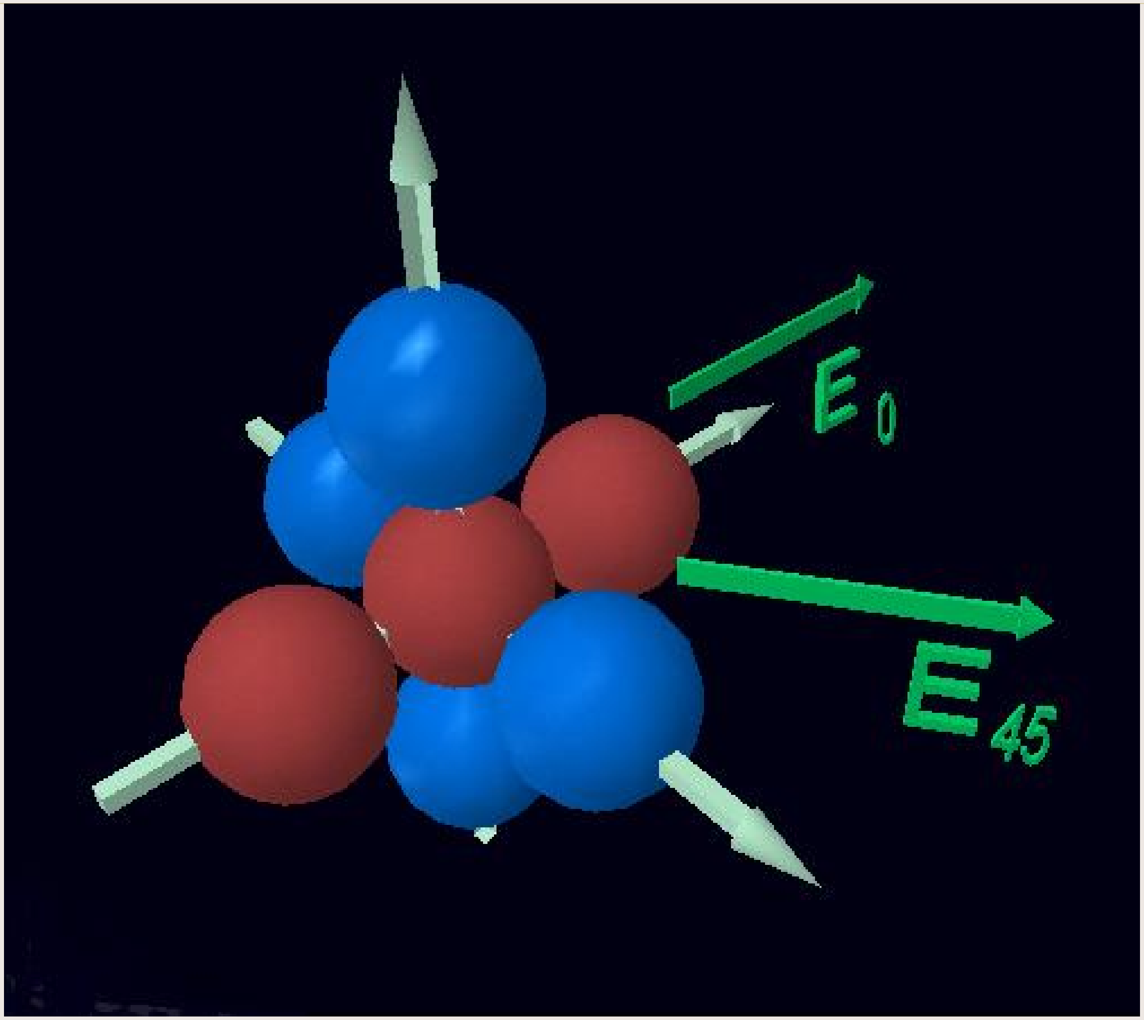


FIG. 1. The ratios of atomic EDMs for the confined and isolated atoms (suppression factor) as a function of cavity radius. The upper and lower sets of two curves are obtained with the DHF and RRPA methods, respectively. EDMs induced by P,T—odd semileptonic interactions are shown as solid and dashed lines, while EDMs due to the Schiff moment—as dotted and dashed-dotted lines. The heavy dot marks our final results for liquid Xe.

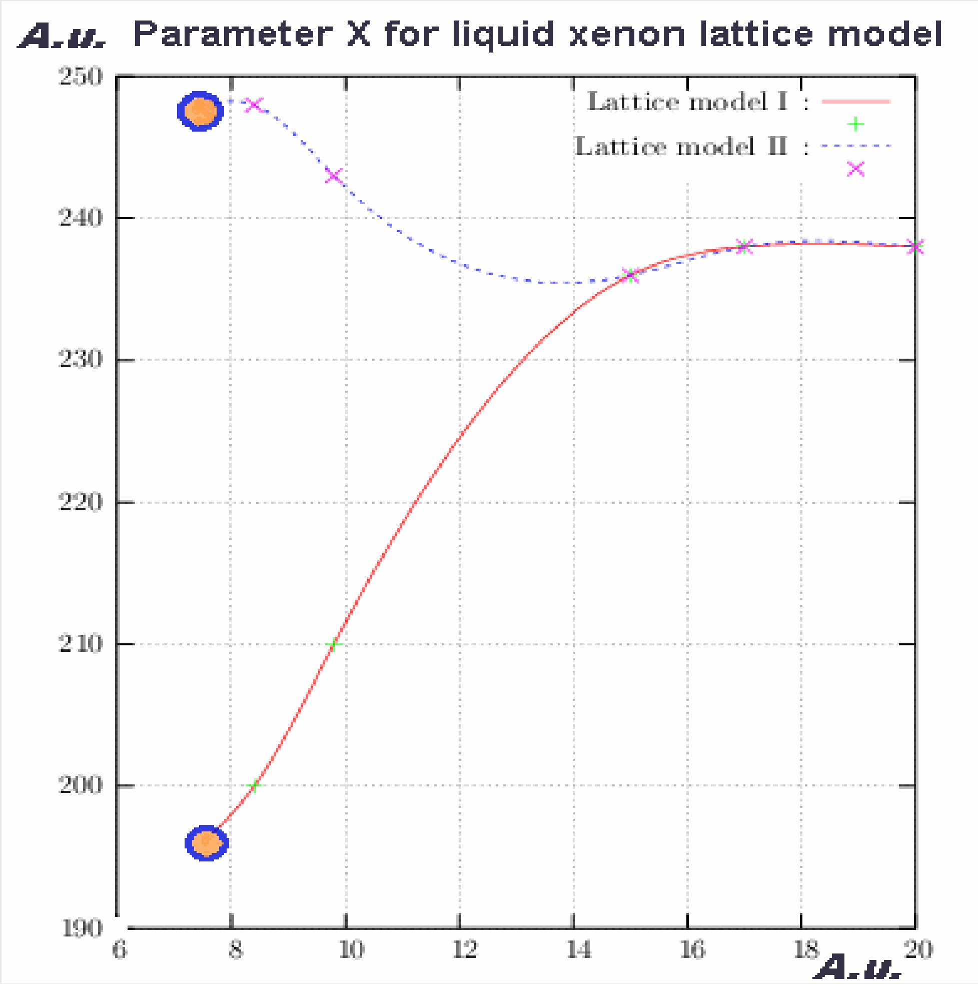
Lattice Model of Liquid Xenon I



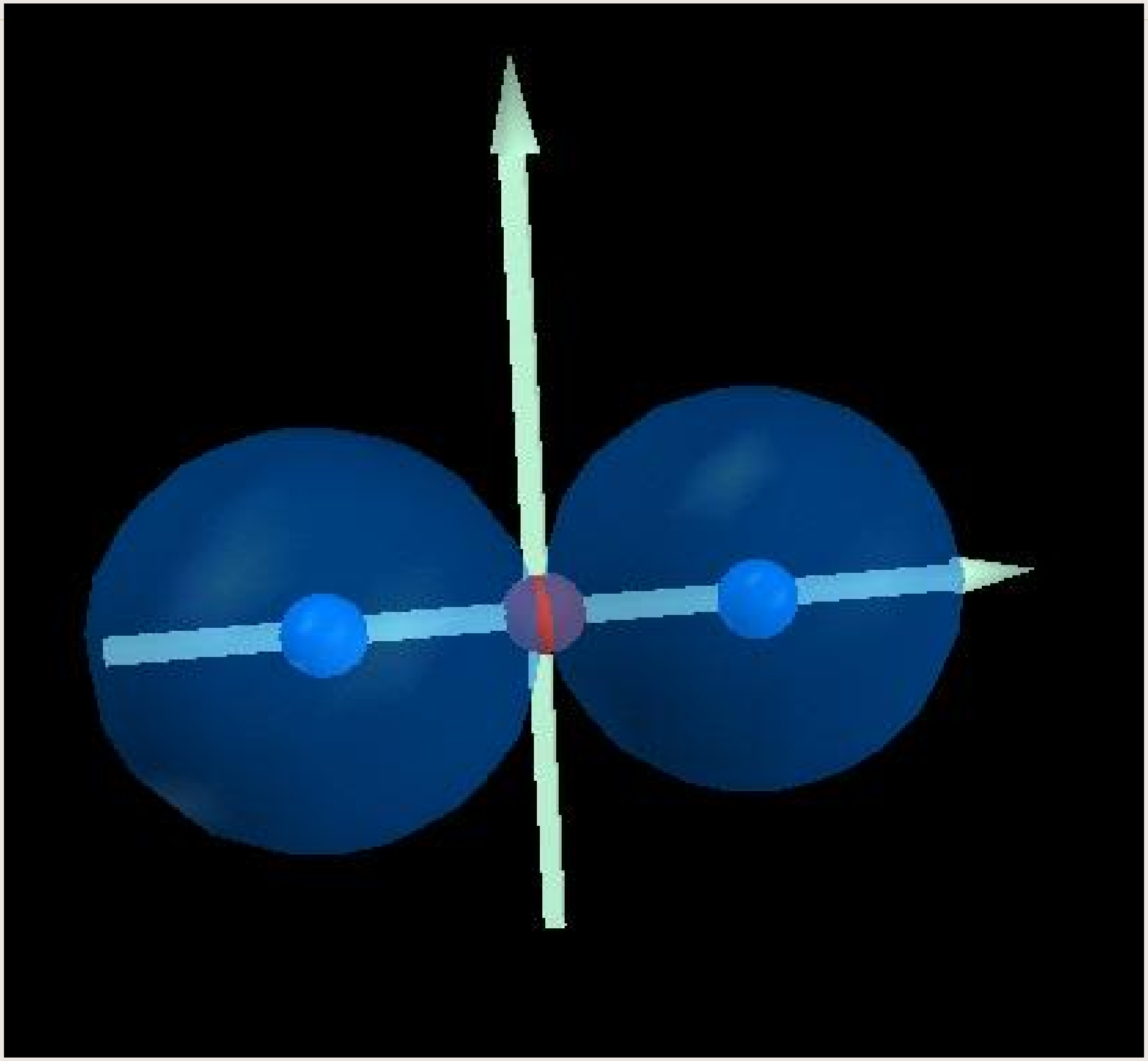
Lattice Model of Liquid Xenon II



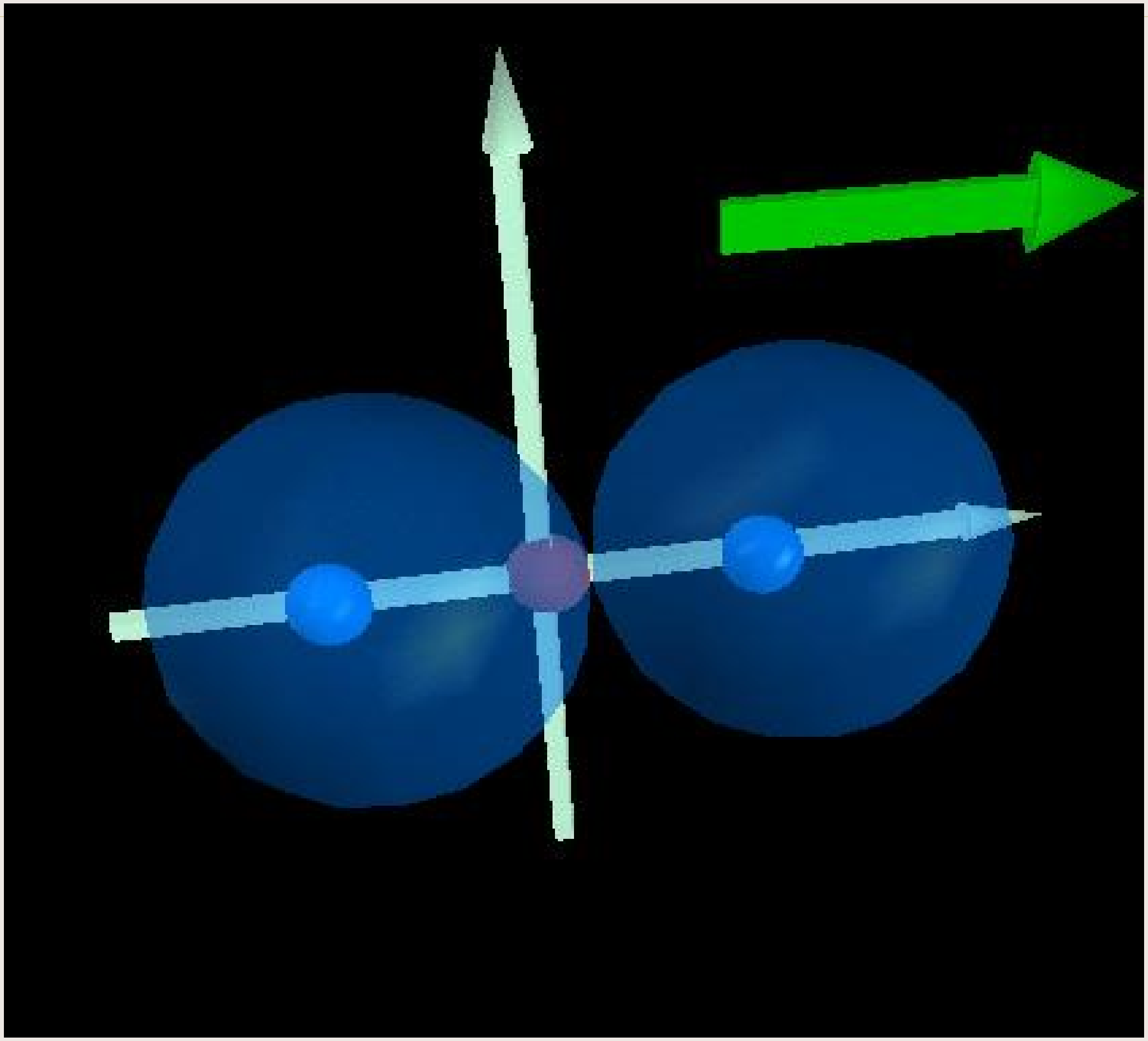
Lattice Model of Liquid Xenon



Lattice Model of Liquid Xenon



Lattice Model of Liquid Xenon



Thank You!