

# THEORETICAL DEVELOPMENTS OF DIRECT INTEREST TO GROUND STATE NUCLEAR STRUCTURE TOWARDS ACTINIDES AND HEAVIER ELEMENTS

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# WHAT ARE WE INTERESTED IN?

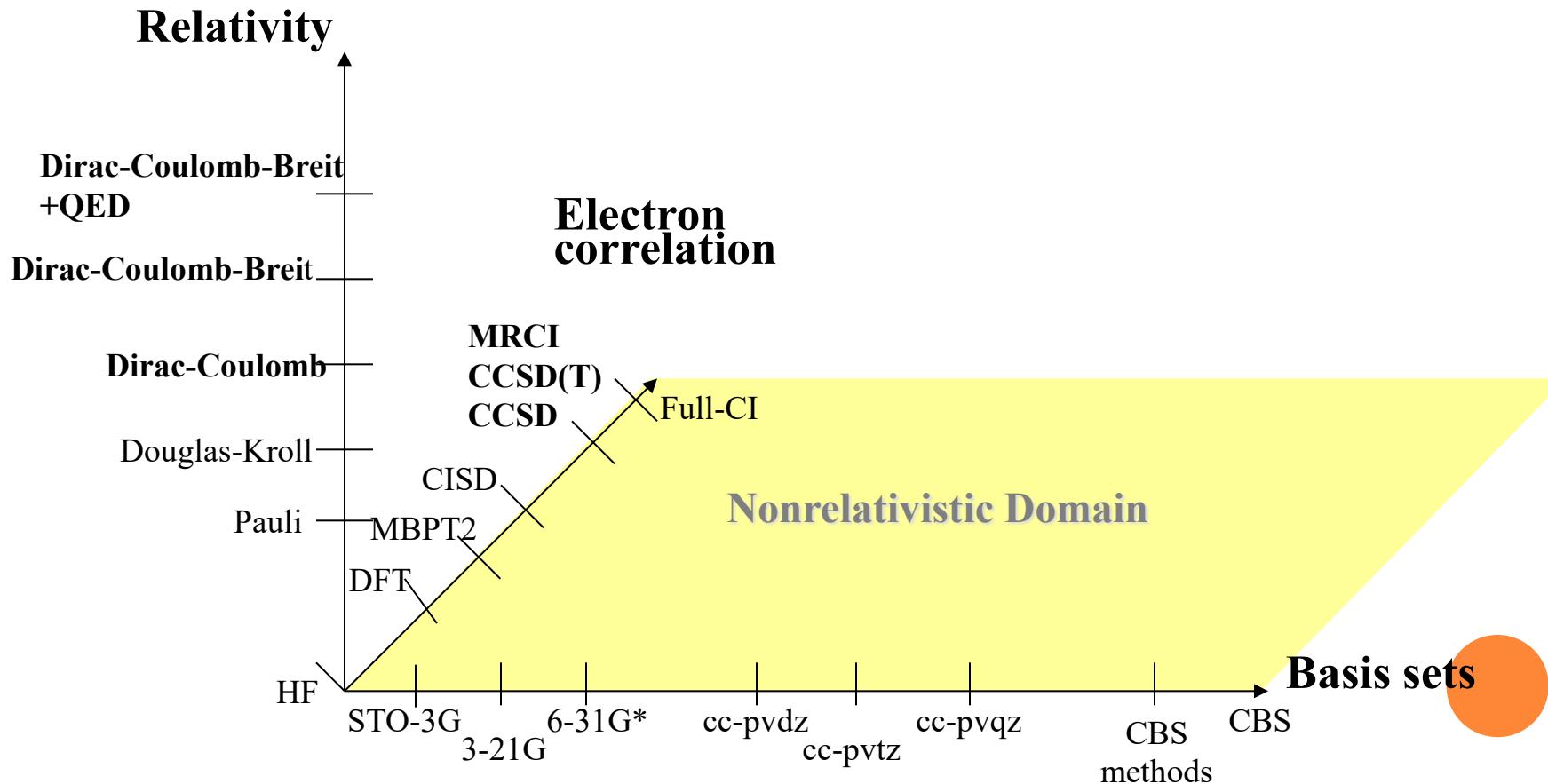
- Theory can provide:
  - Reliable predictions for planning the measurements
  - Interpretation of experiments
  - Theoretical predictions for comparison with the measured values
- Accuracy:
  - High enough to be useful in experiments
  - High enough for prediction and understanding of trends where experiment is not yet available
- Basic atomic properties of heavy and superheavy elements: ionization potentials (IPs), electron affinities (EAs), spectra, polarizabilities, **hyperfine structure**, ...

Realistically, for IPs, EAs and transition energies we obtain accuracy on the order of **a few meV**

What about the hyperfine structure?

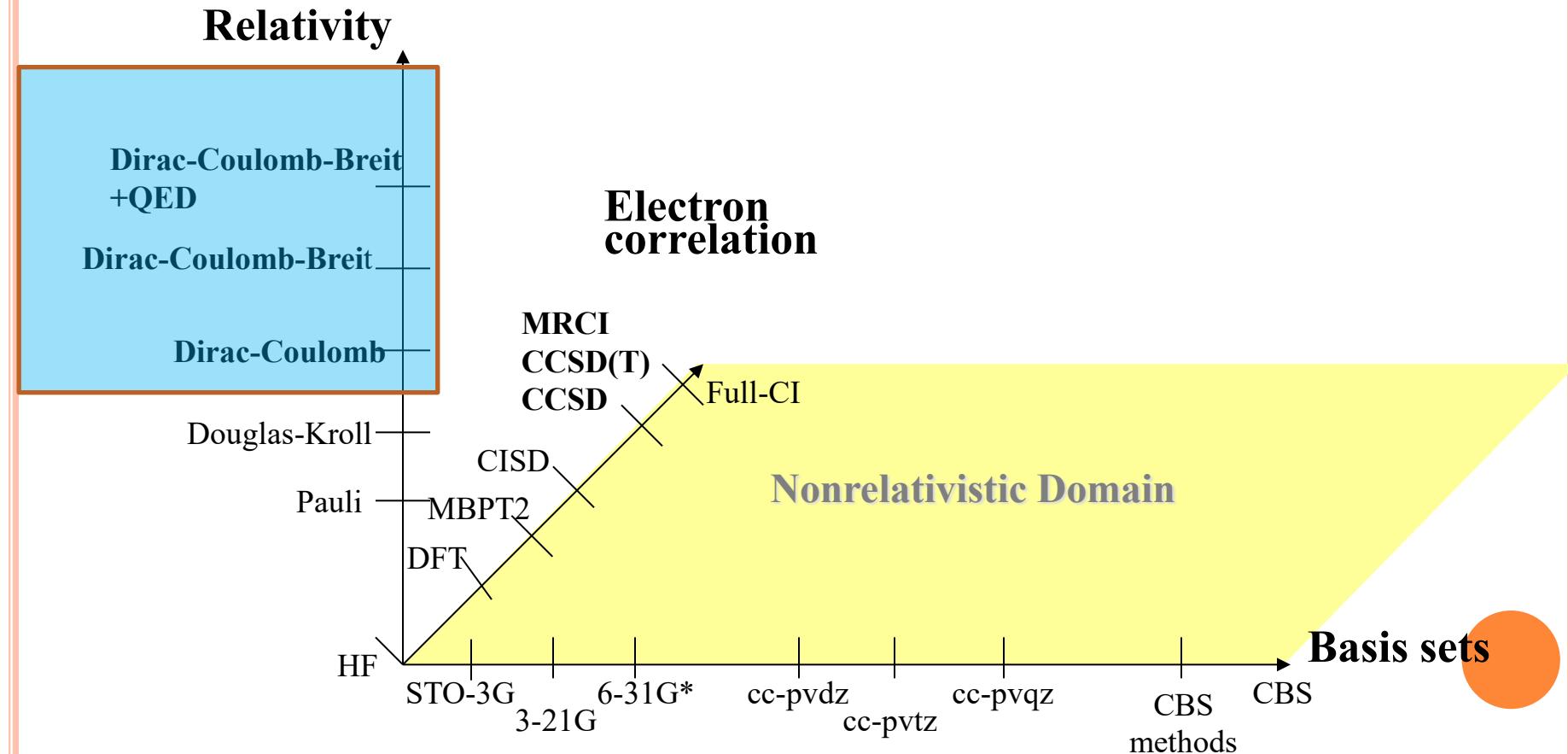


# COMPUTATIONAL METHODS



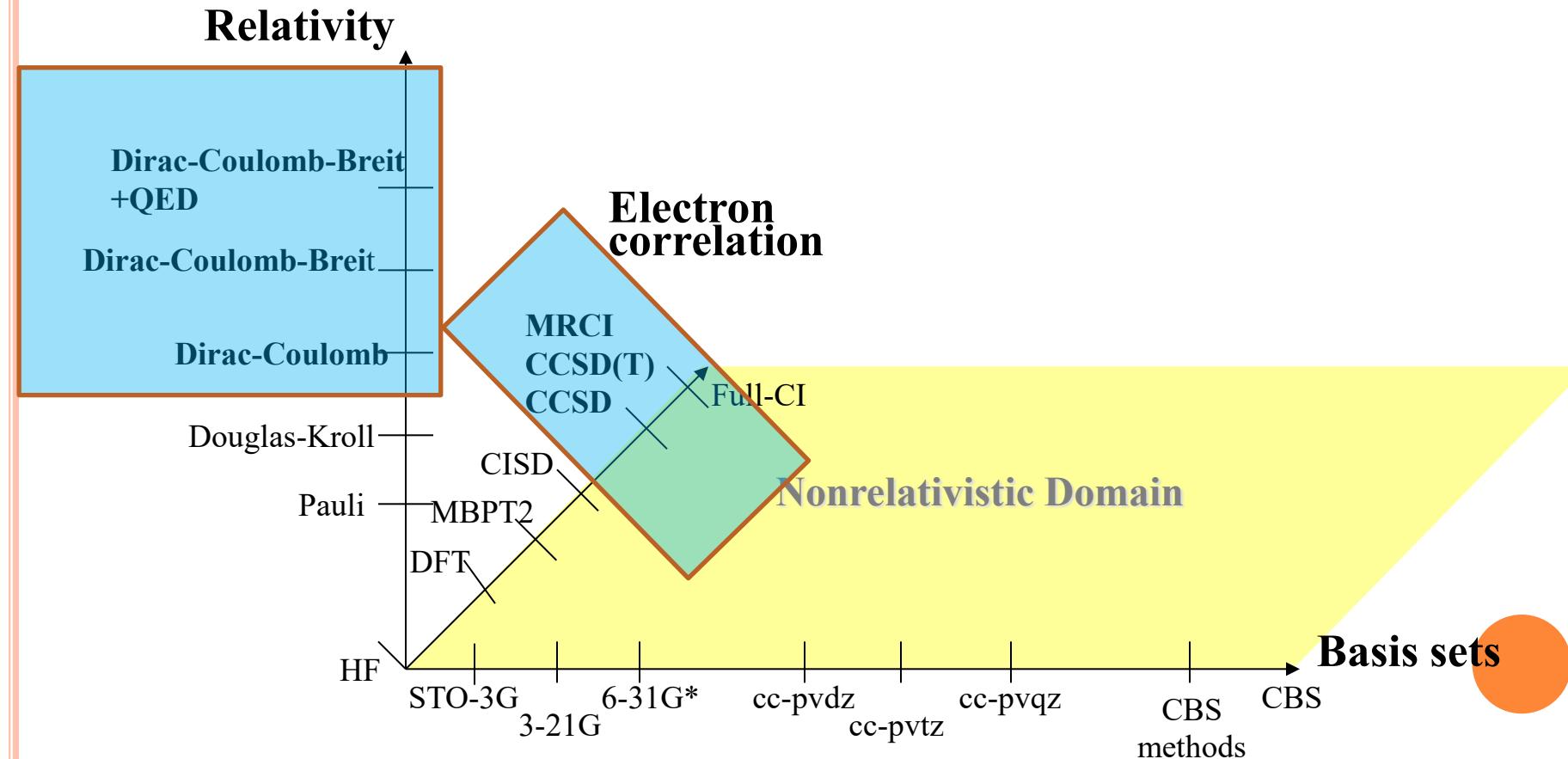
Slide courtesy of P. Schwerdtfeger

# COMPUTATIONAL METHODS



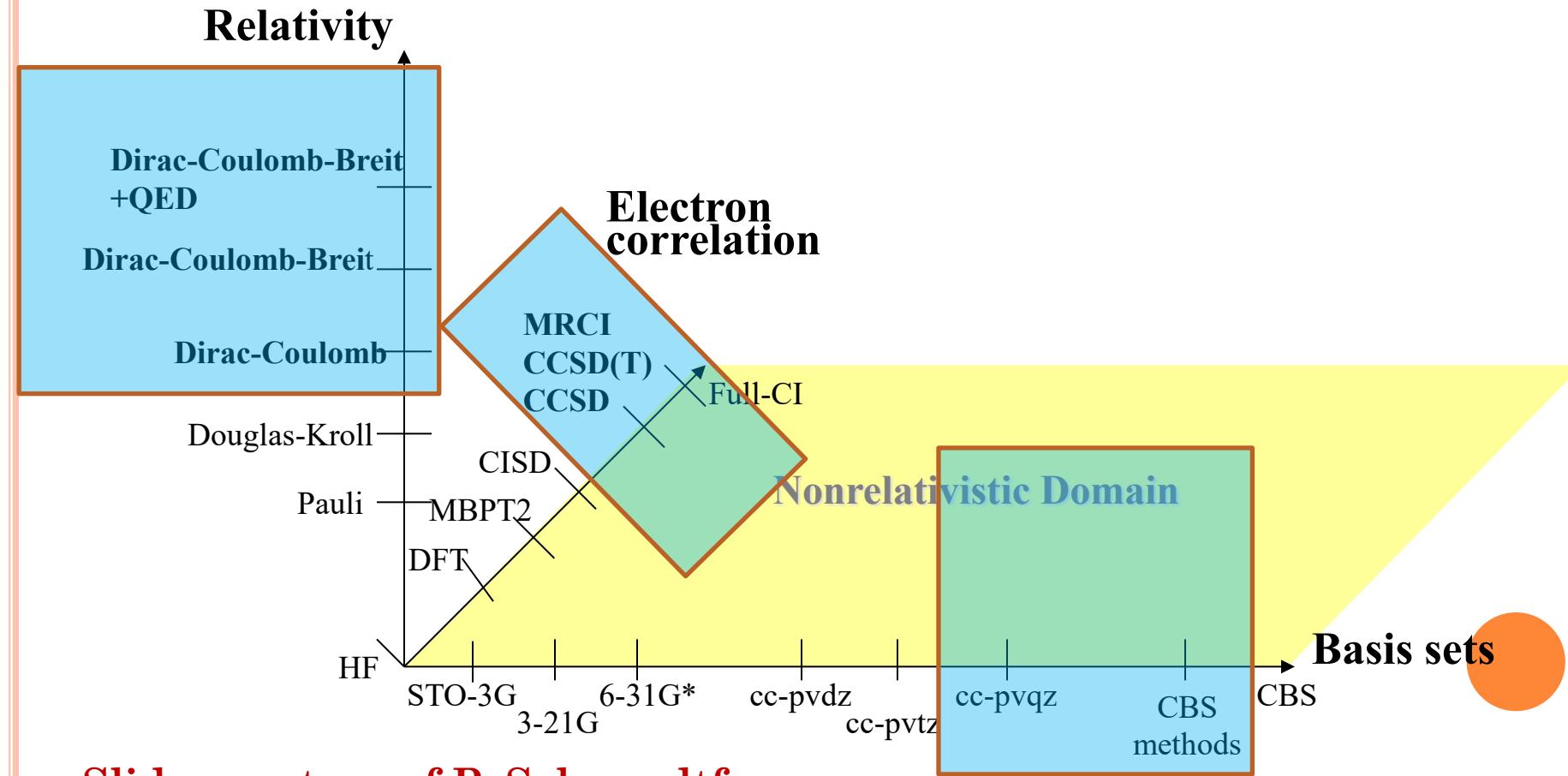
Slide courtesy of P. Schwerdtfeger

# COMPUTATIONAL METHODS



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# COMPUTATIONAL METHODS



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# COMPUTATIONAL METHODS

Relativity

Dirac-Coulomb-Breit  
+QED

Dirac-Coulomb-Breit

Dirac-Coulomb

Douglas-Kroll

Pauli

MBPT2

DFT

HF  
STO-3G  
3-21G  
6-31G\*

Electron correlation

MRCI  
CCSD(T)  
CCSD

CISD

Full-CI

Accuracy comes with a price ☹

Nonrelativistic Domain

cc-pvqz  
CBS  
methods

Basis sets

# RELATIVISTIC FRAMEWORK

- 4-c Dirac-Coulomb-(Breit) Hamiltonian:

$$H_{DCB} = \sum_i h_D(i) + \sum_{i < j} (1/r_{ij} + B_{ij}),$$
$$h_D(i) = c\alpha_i \cdot \mathbf{p}_i + c^2 \beta_i + V_{nuc}(i)$$

- $\alpha_i, \beta_i$  - four dimensional Dirac matrices
- $V_{nuc}$  - nuclear attraction operator; finite nucleus model (hard sphere, Gaussian or Fermi charge distribution)
- $B_{ij} = -\frac{1}{2r_{ij}} [\alpha_i \cdot \alpha_j + (\alpha_i \cdot \mathbf{r}_{ij})(\alpha_j \cdot \mathbf{r}_{ij})/r_{ij}^2]$ : Breit term, higher order corrections (QED) are possible
- 4 component wave functions:

$$\Psi = \begin{pmatrix} \Psi^L \\ \Psi^S \end{pmatrix}$$



# RELATIVISTIC COUPLED CLUSTER

- An extremely powerful method for treatment of electron correlation
- Exponential representation of the wave operator:

$$\Psi = \exp(S)\Psi_0 = \left(1 + S + \frac{S^2}{2!} + \dots\right) \Psi_0$$

- Here,  $S$  is the excitation operator, usually truncated at  $S_2$ :

$$S = \boxed{S_1 + S_2} + \dots + S_N; \quad S_1 = \sum_{ia} s_i^a a_a^\dagger a_i; \quad S_2 = \sum_{ijab} s_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

- Coupled cluster equations:

$$\text{CCSD: } \Psi_{\text{CCSD}} = \exp(S_1 + S_2) |\Phi_0\rangle.$$

$$\langle \Phi_0 | (H - E_{\text{CCSD}}) \exp(S_1 + S_2) |\Phi_0\rangle = 0$$



# COUPLED CLUSTER METHODS

- **Single reference coupled cluster with single, double, and perturbative triple excitations – SRCCSD(T)**

Closed shell systems/systems with one dominant configuration

Ground state and lowest excited states

- **Multi reference coupled cluster, e.g., Fock space coupled cluster (FSCC)**

Open shell systems, systems of multireference character

Ground state and excited states (many transition energies)



# FOCK SPACE COUPLED CLUSTER

- Solve HF equations for closed shell reference state, then add/remove electrons to reach the state of interest
- Divide the function space into model space  $\mathbf{P}$  and a virtual space  $\mathbf{Q} = \mathbf{1} - \mathbf{P}$ .
- Define an effective Hamiltonian:

$$H_{eff} = PH\Omega P,$$

$$\Omega = \mathbf{1} + \chi = \{\exp(S)\} = \mathbf{1} + S + \frac{1}{2}\{S^2\} + \dots$$

$S$  defined wrt closed shell reference determinant; partitioned according to the number of valence holes ( $\mathbf{n}$ ) and valence particles ( $\mathbf{m}$ ) ( $n+m \leq 2$ ):

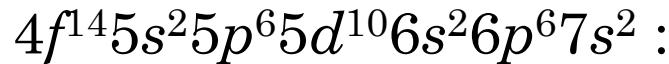
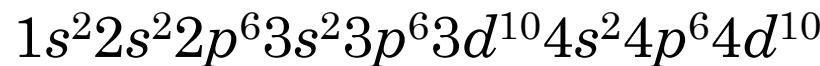
$$S = \sum_{m,n} S^{(n,m)} = S^{(0,0)} + S^{(0,1)} + S^{(1,0)} + \dots$$

- The resulting FSCC equations:

$$Q[S^{(n,m)}, H_0]P = Q(\overline{V\Omega} - \overline{\chi PV\Omega})^{(n,m)}P$$

# EXAMPLE: SPECTRUM OF RA

Ground state:



Periodic Table of the Elements																							
GROUP		VIII																					
IA	IIA	IIIA			IVB		VB		VIB		VIIB		IIB		IIIB		IVB	VB	VIB	VIIB			
1 H	2 He	3 Li	4 Be	11 Na	12 Mg	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
2 He		3 Li	4 Be	11 Na	12 Mg	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
		5 B	6 C	7 N	8 O	9 F	10 Ne	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar										
		19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
		37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe				
		55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn				
		87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Uub										
		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu							
		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr							



- Solve DHF equations
- Correlate closed shell doubly ionized reference state



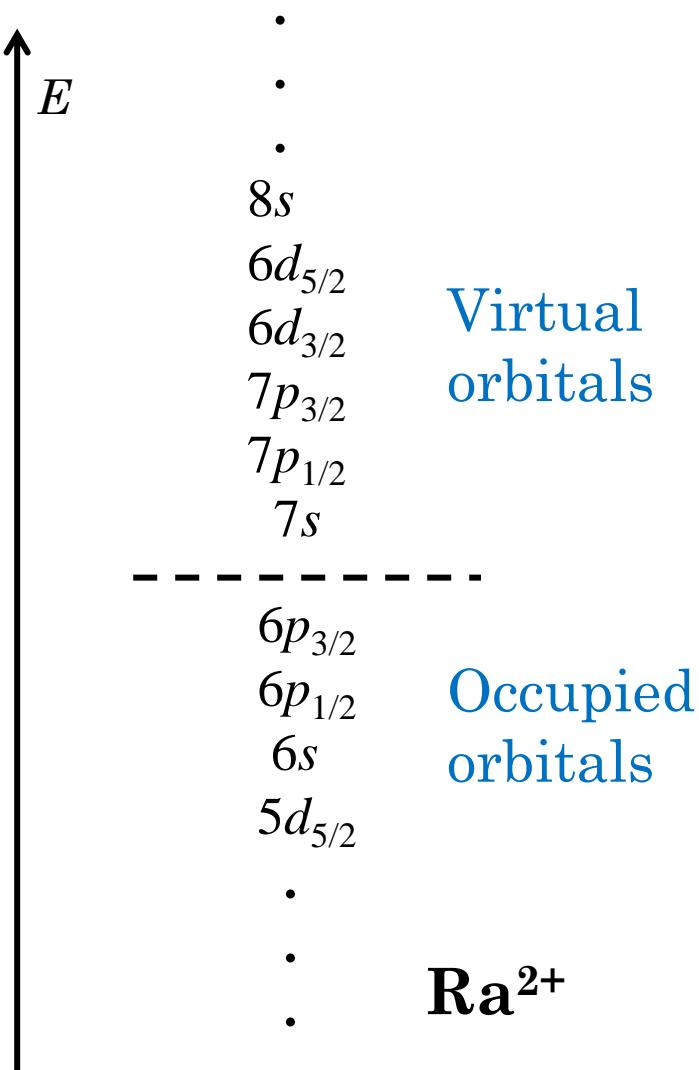
- Add an electron
- Recorrelate



- Add an electron
- Recorrelate



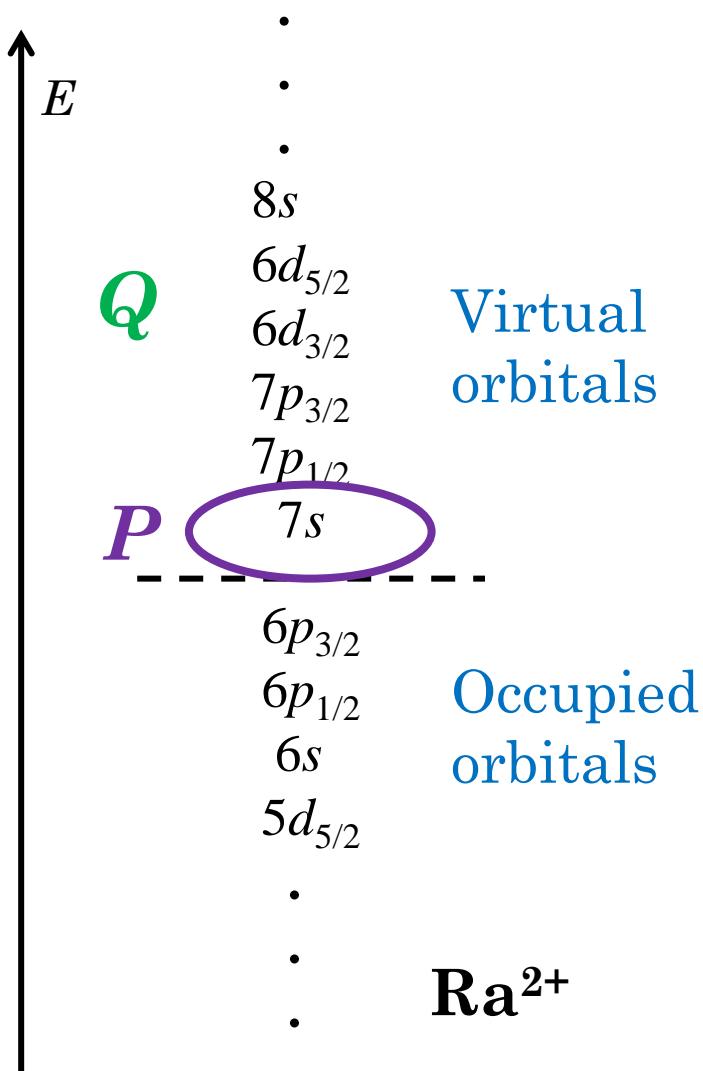
# SPECTRUM OF Ra: MODEL SPACE



**Neutral Ra (NIST):**

Configuration	Term	J	Level(cm <sup>-1</sup> )	Ref.
$7s^2$	$^1S$	0	0.00	M58
$7s7p$	$^3P^o$	0	13078.44	M58
		1	13999.38	M58
		2	16688.54	M58
$7s6d$	$^3D$	1	13715.85	M58
		2	13993.97	M58
		3	14707.35	M58
$7s6d$	$^1D$	2	17081.45	M58
$7s7p$	$^1P^o$	1	20715.71	M58
$7s8s$	$^3S$	1	26754.05	M58
$6d7p$	$^3F^o$	2	28038.05	M58
		3	30117.78	M58
		4	32367.78	M58
$6d7p$	$^1D^o$	2	30918.14	M58
$7s8p$	$^3P^o$	0	31085.88	M58
		1	31563.29	M58
		2	31874.44	M58
Ra II ( ${}^2S_{1/2}$ ) Limit 42573.36 AWT80				

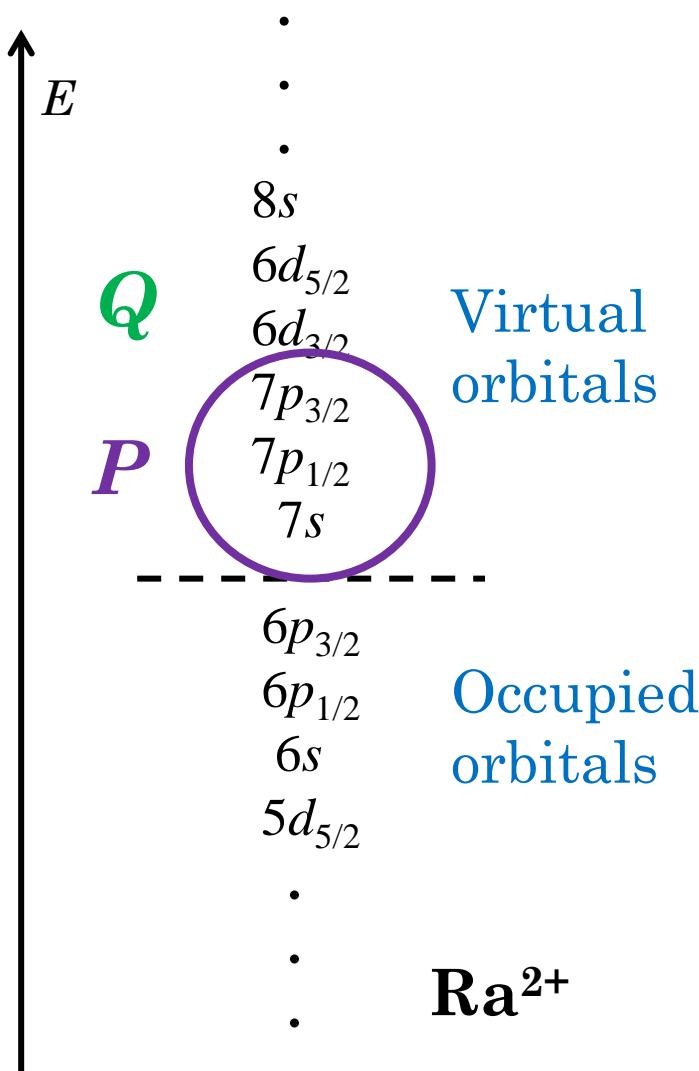
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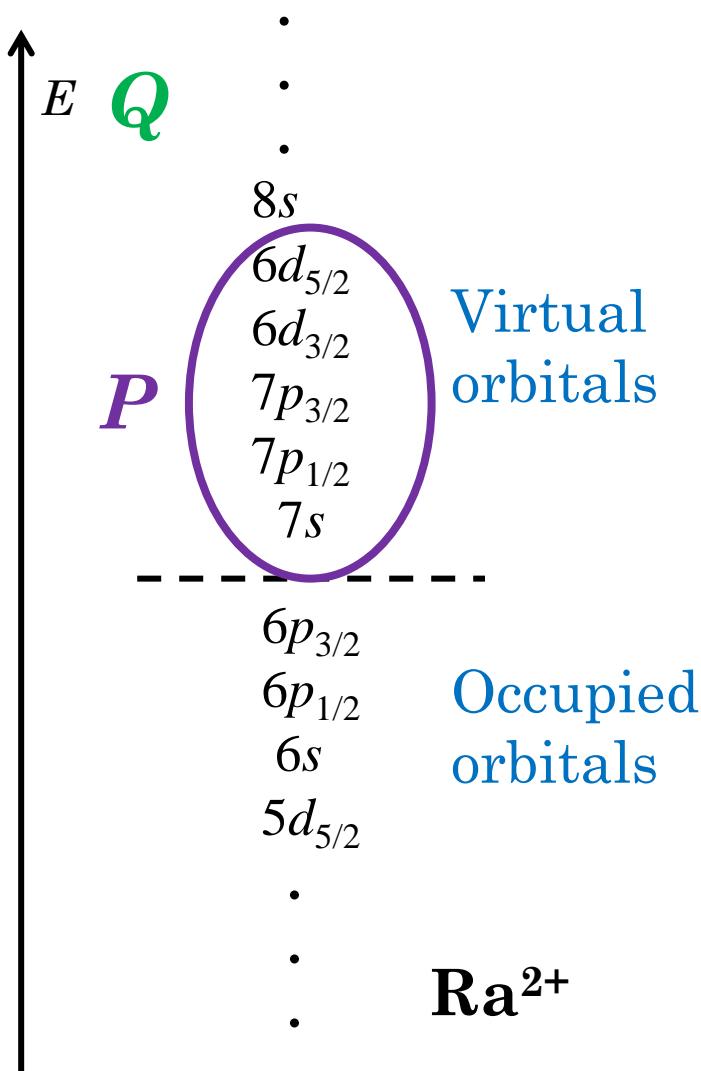
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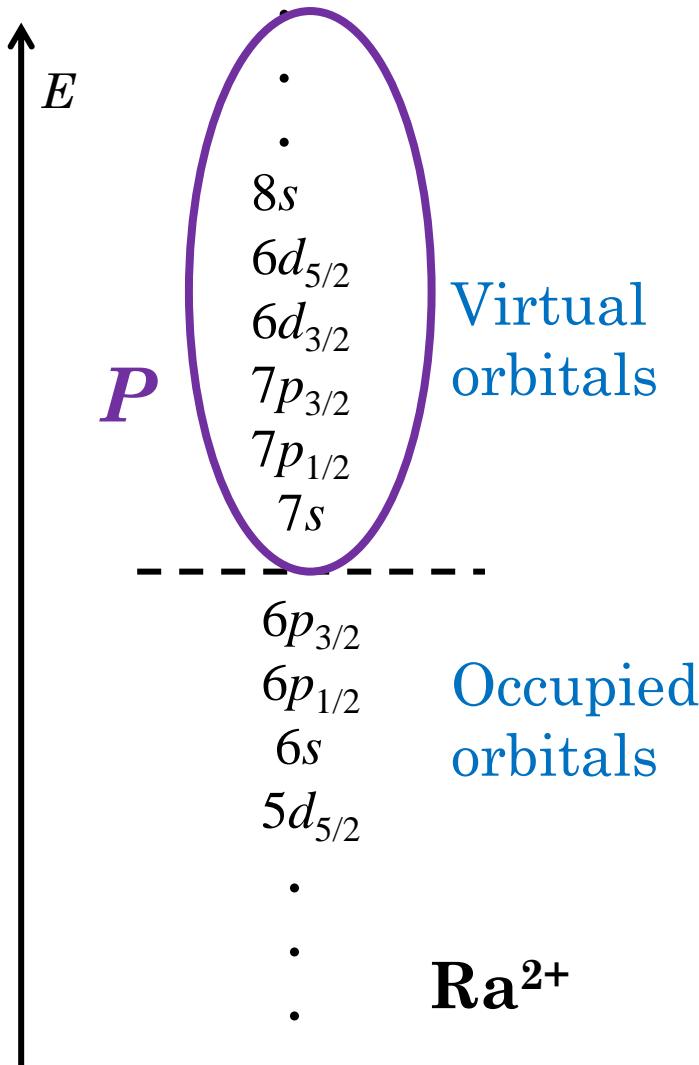
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Ra II ( ${}^2S_{1/2}$ )		Limit	42573.36	AWT80

# MANY ENERGIES IN A SINGLE CALCULATION

**Ra<sup>2+</sup>: ground state energy**

Configuration	Term	J	Level(cm <sup>-1</sup> )	Ref.
7s	<sup>2</sup> S	1/2	0.00	M58
6d	<sup>2</sup> D	3/2	12084.38	M58
		5/2	13743.11	M58
7p	<sup>2</sup> P°	1/2	21351.20	M58
		3/2	26208.86	M58
8s	<sup>2</sup> S	1/2	43405.01	M58
7d	<sup>2</sup> D	3/2	48744.04	M58
		5/2	49240.48	M58
5f	<sup>2</sup> F°	5/2	48987.98	M58
		7/2	49272.31	M58
8p	<sup>2</sup> P°	1/2	50606.01	M58
		3/2	52392.05	M58
9s	<sup>2</sup> S	1/2	59165.23	M58
Ra III (1S <sub>0</sub> )	<b>Limit</b>		<b>81842.31</b>	M58

**Neutral Ra :**

Configuration	Term	J	Level(cm <sup>-1</sup> )	Ref.
7s <sup>2</sup>	<sup>1</sup> S	0	0.00	M58
7s7p	<sup>3</sup> P°	0	13078.44	M58
		1	13999.38	M58
		2	16688.54	M58
7s6d	<sup>3</sup> D	1	13715.85	M58
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		1	31563.29	M58
		2	31874.44	M58
Ra II (2S <sub>1/2</sub> )	<b>Limit</b>		<b>42573.36</b>	AWT80

# CONFIGURATION INTERACTION (CI)

$$|\Psi\rangle = c_0|\Phi_0\rangle + \sum_{ra} c_a^r |\Phi_a^r\rangle + \sum_{a < b, r < s} c_{ab}^{rs} |\Phi_{ab}^{rs}\rangle + \sum_{r < s < t, a < b < c} c_{abc}^{rst} |\Phi_{abc}^{rst}\rangle + \dots$$

$$\mathbf{Hc} = E\mathbf{c}.$$

- CI is great at treating correlation between the valence electrons, but is not very accurate for core-core and core-valence correlations.
- These missing correlations are included by means of second order many body perturbation theory (MBPT).
- CI+MBPT, many transition energies obtained in a single calculation



	<b>SRCCSD(T)</b>	<b>FSCC</b>	<b>CI+MBPT</b>
Systems	Closed shell/ single conf.	Open shell, multiconf.	Open shell, multiconf.
States	Ground and low excited	Many excited states	Many excited states
Valence particles/holes	No strict limit	Up to 2	No strict limit
Excitations	Single, double, perturbative triple	Single and double	Single, double, triple
Which parameters?	FS	$B$ , FS	$A$ , $B$ , FS
Program	DIRAC15	DIRAC15, TRAFS-3C	AMBiT

- **TRAFS-3C:** Tel-Aviv Relativistic Atomic Fock-Space coupled cluster
- **DIRAC15:** DIRAC, a relativistic *ab initio* electronic structure program, release 2015
- **AMBiT**, developed by Julian Berengut, UNSW



# APPLICATIONS



# HYPERFINE STRUCTURE CONSTANTS: $A$

○  $^{173}\text{Yb}$  [ $6s^2\ 1S_0$ ]

		E (Exp.)	$A$ (Exp.)	$A$ (CI+MBPT)
$6s6p$	$^3P_0$	17089		
	$^3P_1$	17806	-1094	-1099
	$^3P_2$	19540	-738	-753
$6s5d$	$^1P_1$	26118	59	184
	$^3D_1$	24489	563	623
	$^3D_2$	24752	-362	-371
	$^3D_3$	25271	-430	-427
	$^1D_2$	27678	100	135
	$\Delta A$			36

\*Energies -  $\text{cm}^{-1}$ ,  $A$  - MHz

\*\*  $^{173}\text{Yb}$ ,  $I=5/2$   $\mu=-0.6776 \mu_N$



# HYPERFINE STRUCTURE CONSTANTS: $A$

- $^{253}\text{No}$  [ $7s^2 \ ^1\text{S}_0$ ]

		E (FSCC)***	$A$ (CI+MBPT)
$7s7p$	$^3\text{P}_0$	19028	
	$^3\text{P}_1$	20605	4439
	$^3\text{P}_2$	25527	2362
	$^1\text{P}_1$	30054 ( <b>29961</b> )	-1650
$7s6d$	$^3\text{D}_1$	28496	2175
	$^3\text{D}_2$	28935	1372
	$^3\text{D}_3$	30040	1443
	$^1\text{D}_2$	33071	-704

\*Energies -  $\text{cm}^{-1}$ ,  $A$  – MHz

\*\*  $I=9/2$   $\mu=\mu_N$

\*\*\* A.Borschevsky *et al.*, PRA **75**, 042514 (2007)

\*\*\* Exp. :Laatiaoui *et al.*, Nature 2016  
(doi:10.1038/nature19345)



# HYPERFINE STRUCTURE CONSTANTS: $A$

- $^{175}\text{Lu}$  [ $6s^2 6d\ ^2\text{D}_{3/2}$ ]

		E (Exp.)	$A$ (Exp.)	$A$ (CI+MBPT)
$6s^2 5d$	$^2\text{D}_{3/2}$	0	195	167
	$^2\text{D}_{5/2}$	1994	149	60
$6s^2 6p$	$^2\text{P}_{1/2}$	4136		1303
	$^2\text{P}_{3/2}$	7476	221	202
$6s^2 7s$	$^2\text{S}_{1/2}$	24126	1758	1903

\*Energies -  $\text{cm}^{-1}$ ,  $A$  - MHz

\*\*  $I=7/2$   $\mu=2.232\mu_N$



# HYPERFINE STRUCTURE CONSTANTS: $A$

- $^{255}\text{Lr}$  [ $7s^2 7p\ ^2\text{P}_{1/2}$ ]

		E (FSCC)***	$A$ (CI+MBPT)
$6s^2 5d$	$^2\text{D}_{3/2}$	1436	-62
	$^2\text{D}_{5/2}$	5106	90
$6s^2 6p$	$^2\text{P}_{1/2}$	0	2561
	$^2\text{P}_{3/2}$	8413	-4
$6s^2 7s$	$^2\text{S}_{1/2}$	20118	2257

\*Energies -  $\text{cm}^{-1}$ ,  $A$  - MHz

\*\*  $I=7/2$   $\mu=\mu_N$

\*\*\* A. Borschevsky *et al.*, EPJD **45**, 115 (2007)



# HYPERFINE STRUCTURE CONSTANTS: $B$

- FSCC: finite field approach:

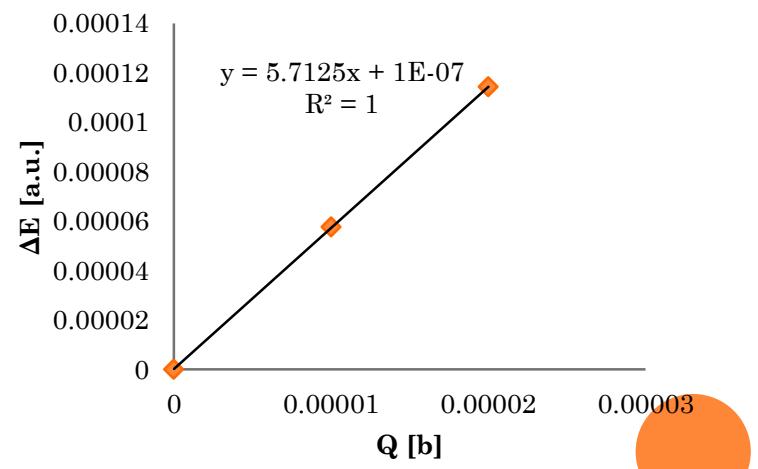
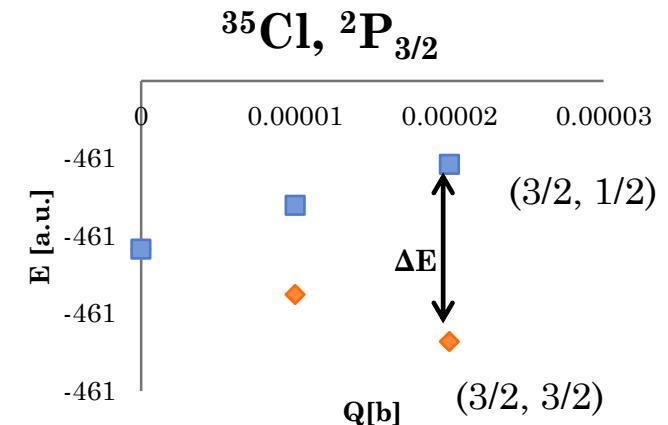
$$B[\text{MHz}] = 234.96 \cdot Q[\text{b}] \cdot q[\text{a.u.}]$$

$$\hat{H}(Q) = \hat{H}_0 - eqQ/h.$$

$$E(Q) = \langle \Psi(Q) | \hat{H}(Q) | \Psi(Q) \rangle$$

$$= E_0 + Q \left( \frac{dE(Q)}{dQ} \right)_0 + \frac{Q^2}{2} \left( \frac{d^2E(Q)}{dQ^2} \right)_0 + \dots$$

$$\left. \frac{dE(Q)}{dQ} \right|_{Q=0} = -\frac{e}{h} \langle \Psi_0 | \hat{q}_{zz} | \Psi_0 \rangle.$$



$$B(\text{FSCC}) = -54.36 \text{ MHz}$$

$$B(\text{Exp.}) = -55.35 \text{ MHz}$$

# HYPERFINE STRUCTURE CONSTANTS: $B$

○  $^{173}\text{Yb}$  [ $6s^2\ 1S_0$ ]

		E (Exp.)	$B$ (Exp.)	$B$ (FSCC)
$6s6p$	$^3P_0$	17089		
	$^3P_1$	17806	-838	-827
	$^3P_2$	19540	1347	1312
	$^1P_1$	26118	744	605
$6s5d$	$^3D_1$	24489	303	335
	$^3D_2$	24752	436	482
	$^3D_3$	25271	771	909
	$^1D_2$	27678	1153	1115
$\Delta A$				57

\*Energies -  $\text{cm}^{-1}$ ,  $B$  - MHz

\*\*  $^{173}\text{Yb}$ ,  $I=5/2$   $Q=2.8$



# HYPERFINE STRUCTURE CONSTANTS: $B$

- $^{253}\text{No}$  [ $7s^2 \ ^1\text{S}_0$ ]

		E (FSCC)***	$B$ (FSCC)
7s7p	$^3\text{P}_0$	19028	
	$^3\text{P}_1$	20605	-708
	$^3\text{P}_2$	25527	878
	$^1\text{P}_1$	30054 ( <b>29961</b> )	465
7s6d	$^3\text{D}_1$	28496	246
	$^3\text{D}_2$	28935	374
	$^3\text{D}_3$	30040	546
	$^1\text{D}_2$	33071	679

\*Energies -  $\text{cm}^{-1}$ ,  $B$  - MHz

\*\*  $I=9/2$   $Q=1$  b

\*\*\* A.Borschevsky *et al.*, PRA **75**, 042514 (2007)

\*\*\* Exp. :Laatiaoui *et al.*, Nature 2016  
(doi:10.1038/nature19345)

# HYPERFINE STRUCTURE CONSTANTS: $B$

- $^{175}\text{Lu}$  [ $6s^2 6d\ ^2\text{D}_{3/2}$ ]

		E (Exp.)	$B$ (Exp.)	$B$ (FSCC)
$6s^2 5d$	$^2\text{D}_{3/2}$	0	1511	1599
	$^2\text{D}_{5/2}$	1994	1865	1947
$6s^2 6p$	$^2\text{P}_{1/2}$	4136		
	$^2\text{P}_{3/2}$	7476	2091	2120
$6s^2 7s$	$^2\text{S}_{1/2}$	24126		

\*Energies -  $\text{cm}^{-1}$ ,  $B$ - MHz

\*\*  $I=7/2$   $Q=3.44$  B



# HYPERFINE STRUCTURE CONSTANTS: $B$

- $^{255}\text{Lr}$  [ $7s^2 7p\ ^2\text{P}_{1/2}$ ]

		E (FSCC)***	$B$ (CI+MBPT)
$6s^2 5d$	$^2\text{D}_{3/2}$	1436	853
	$^2\text{D}_{5/2}$	5106	892
$6s^2 6p$	$^2\text{P}_{1/2}$	0	
	$^2\text{P}_{3/2}$	8413	1018
$6s^2 7s$	$^2\text{S}_{1/2}$	20118	

\*Energies -  $\text{cm}^{-1}$ ,  $A$  - MHz

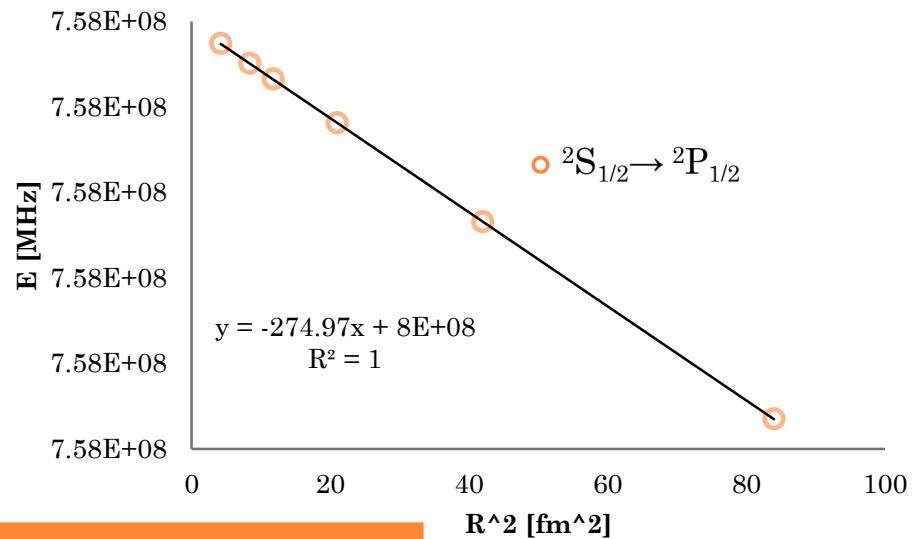
\*\*  $I=7/2$   $\mu=\mu_N$

\*\*\* A. Borschevsky *et al.*, EPJD **45**, 115 (2007)



# FIELD SHIFTS

- Test case: Ca<sup>+</sup>



FS	FS(Exp.)*	FSCC
$^2S_{1/2} \rightarrow ^2P_{1/2}$	-281.8	-277.0
$^2S_{1/2} \rightarrow ^2P_{3/2}$	-284.7	-277.2

\* FS - MHz/fm<sup>2</sup>

\*\* C. Shi *et al.*, arXiv:1608.07572

# FIELD SHIFTS

- Yb [ $6s^2 \ ^1S_0$ ]

	E (Exp.)	FS (Exp.)	FS (FSCC)	FS (CI+MBPT)
$^3P_0$	17089		-9.59	-10.21
$^3P_1$	17806	-11.50	-9.66	-10.28
$^3P_2$	19540		-9.84	-10.44
$^1P_1$	26118	-4.83	-8.67	-9.12

\* Energies -  $\text{cm}^{-1}$ , FS -  $\text{GHz/fm}^2$



# FIELD SHIFTS

- No [  $7s^2 \ ^1S_0$ ]

	E (Exp.)	E (FSCC)	FS (FSCC)	FS (CI+MBPT)
$^3P_0$		19028	-105.5	-113.9
$^3P_1$		20605	-107.8	-114.9
$^3P_2$		25527	-114.6	-121.4
$^1P_1$	29961**	30054***	-98.8	-106.2

\* Energies -  $\text{cm}^{-1}$ , FS - GHz/fm $^2$

\*\* Laatiaoui *et al.*, Nature 2016 (doi:10.1038/nature19345)

\*\*\* Borschevsky *et al.*, PRA 75, 042514 (2007)



# CONCLUSIONS

- Powerful computational approaches ideally suitable for calculation of properties of heavy systems
- Good agreement with experiment where available and reliable predictions. Results obtained in reasonable time
- Versatile approaches, suitable for different types of systems. Depending on the system and on the desired properties we can use the appropriate method, or more than one in parallel
- Successful (and fun) collaborations with experiment
- Work in progress!

