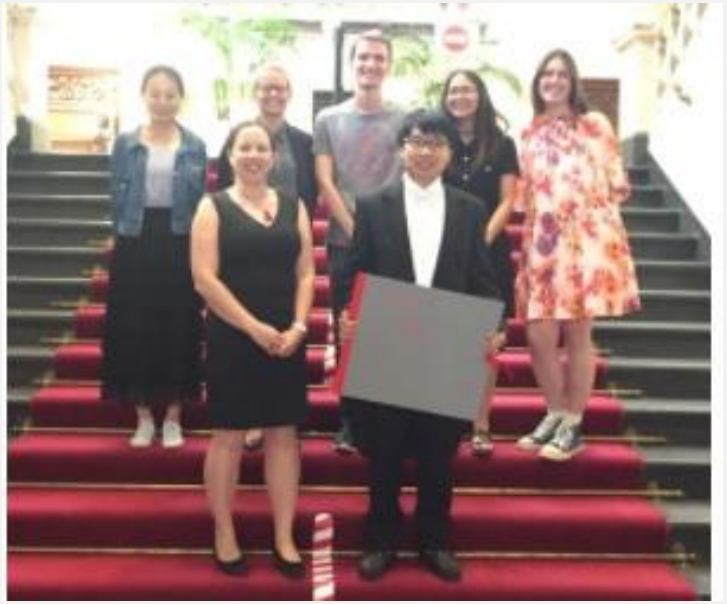
RELATIVISTIC COUPLED CLUSTER: A POWERFUL COMPUTATIONAL TOOL IN SUPPORT OF EXPERIMENTS

A. Borschevsky

university of groningen
faculty of science and engineering
van swinderen institute for particle physics and gravity



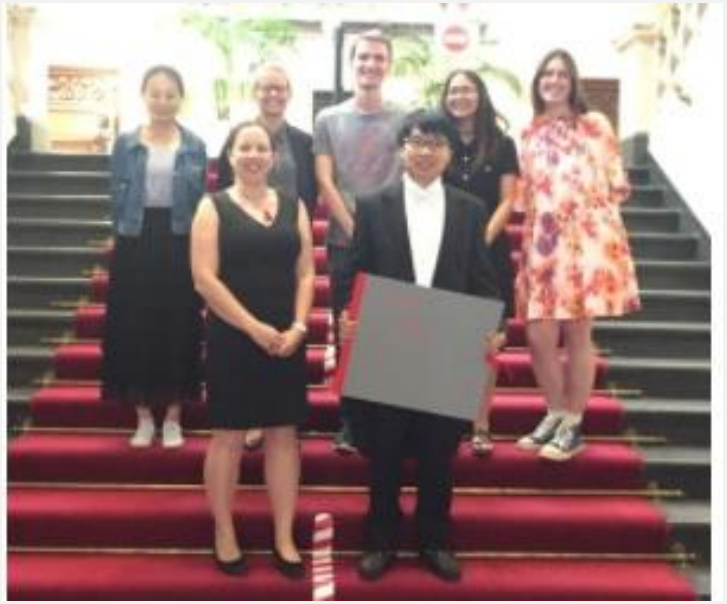
- University of Groningen

<u>Research:</u>

Using state of the art methods from computational chemistry to address fundamental problems in physics:

- Search for new physics with low-energy precision measurements
  - Violation of fundamental symmetries in atoms and in molecules
  - Search for variation of fundamental constants
- Highly accurate calculations of spectra and properties of heavy and superheavy atoms and highly charged ions

Most work done in collaboration with experimental groups



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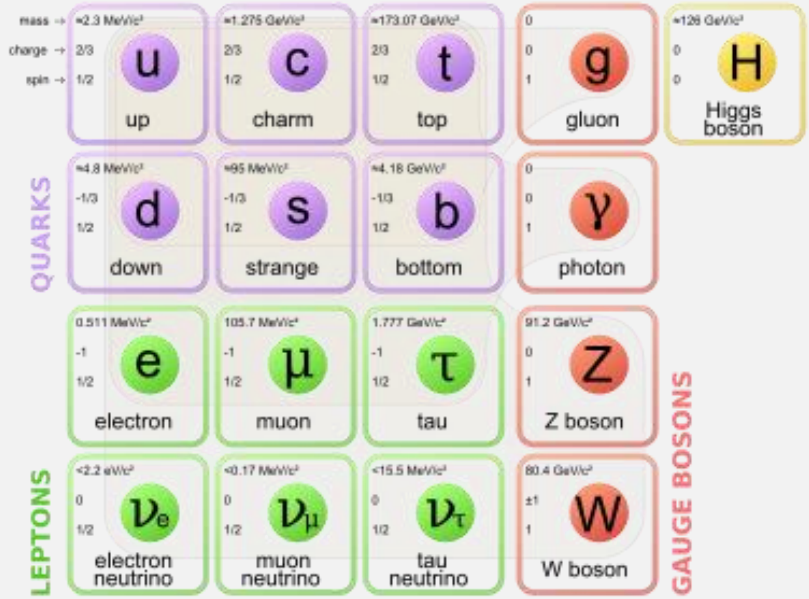
MOTIVATION

Why look for physics beyond the Standard Model (SM)?

- The SM is currently the best fitting physical description of the world around us.
- So far successfully explained the majority of observed natural phenomena and has strong predictive power (Higgs boson, top quark, tau neutrino)
- But… it is incomplete

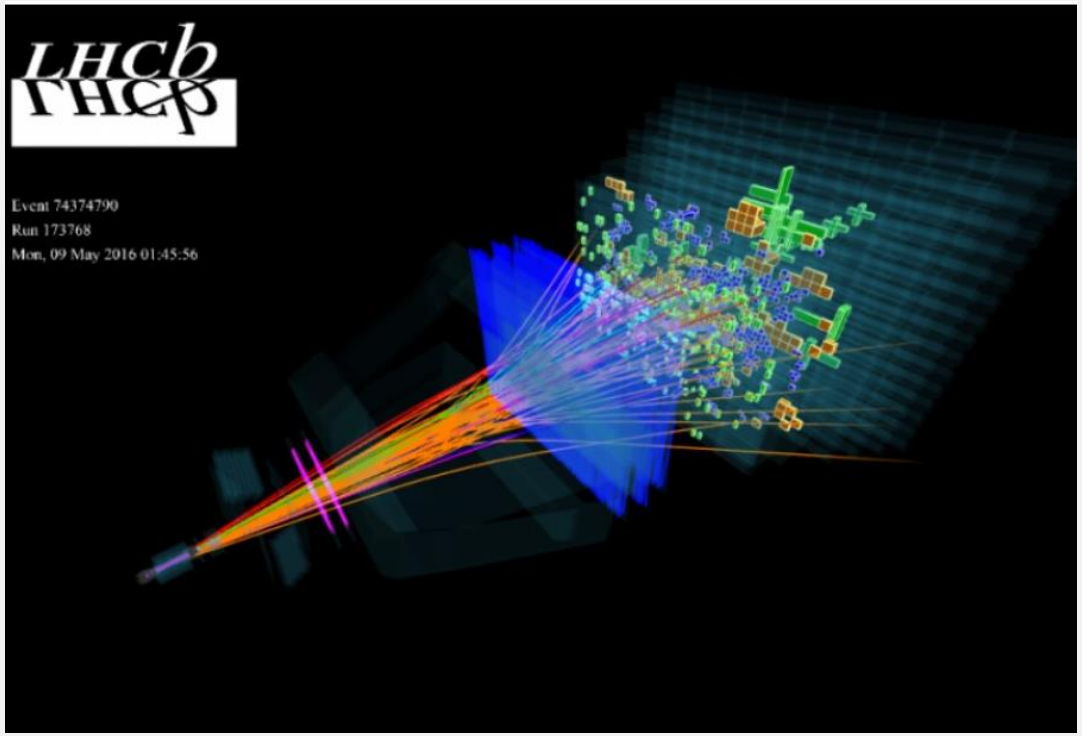


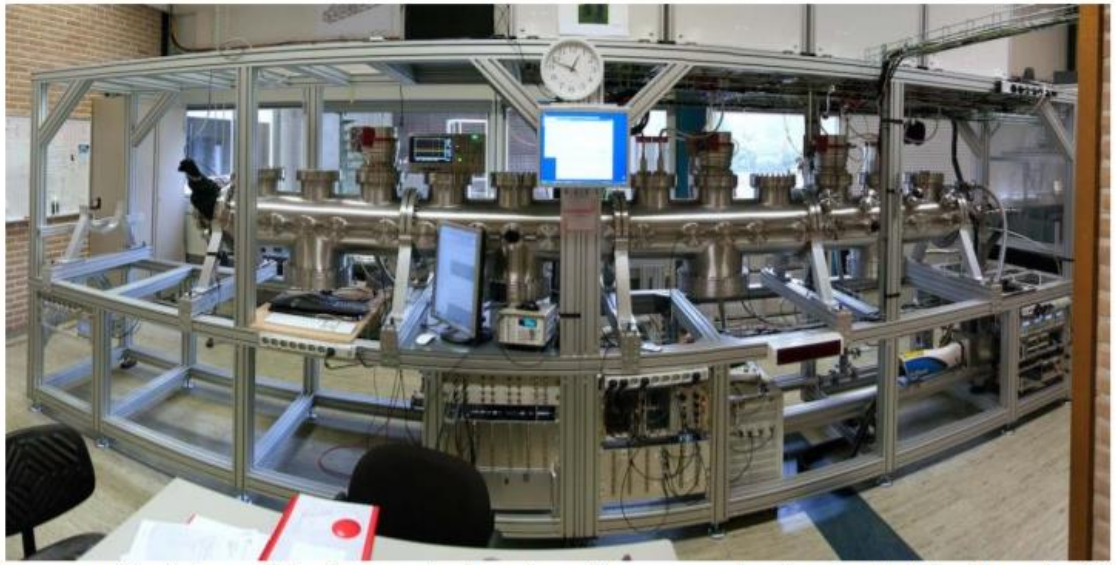
Why look for physics beyond the Standard Model (SM)?

- Extensions to the SM attempt to fill these knowledge gaps.
  - Grand Unified Theories, String Theory, SUSY, …
- These extensions predict new physical phenomena beyond the SM.
  - Variation of fundamental constants (VFC)
  - Violation of fundamental symmetries (*CP*, *P*, *T*)
- (non) discovery of these phenomena allows to discriminate between extensions or new theories.

Why look for physics beyond the SM with atoms and molecules?

- Accelerator research (LHCb, T2K, etc.)
- **Table-top experiments**





A panoramic picture of the four meter long traveling-wave decelerator that has been built in Groningen. It is in use for decelerating packets of the heavy diatomic molecule SrF, which is a prototypical system for the investigation of broken symmetries.

Why look for physics beyond the SM with atoms and molecules?

- **Table-top experiments: promising alternative to high energy research**
  - Versatile, sensitive to different phenomena
    - Parity violation
    - EDMs (electron, hadronic)
    - Variation of fundamental constants
    - Dark matter
    - ..
  - Various enhancement effects→ high sensitivity
  - Small scale
  - (Relatively) inexpensive

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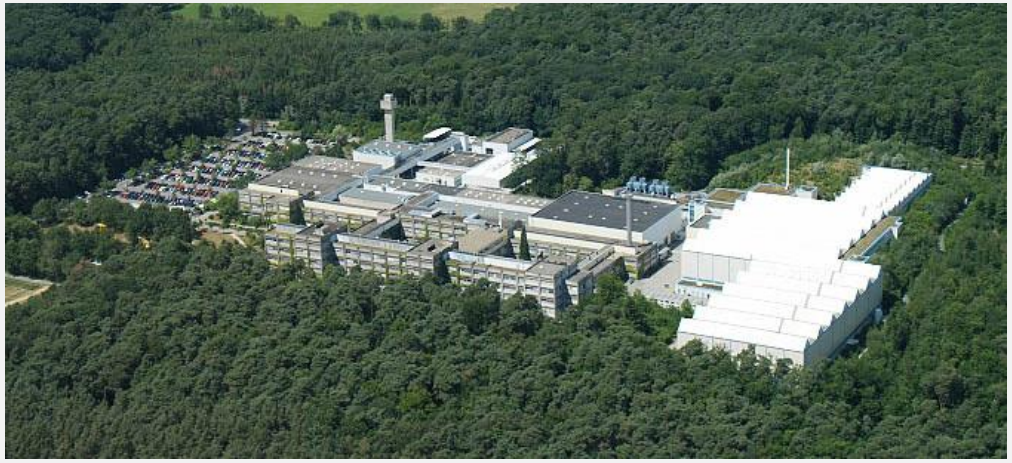
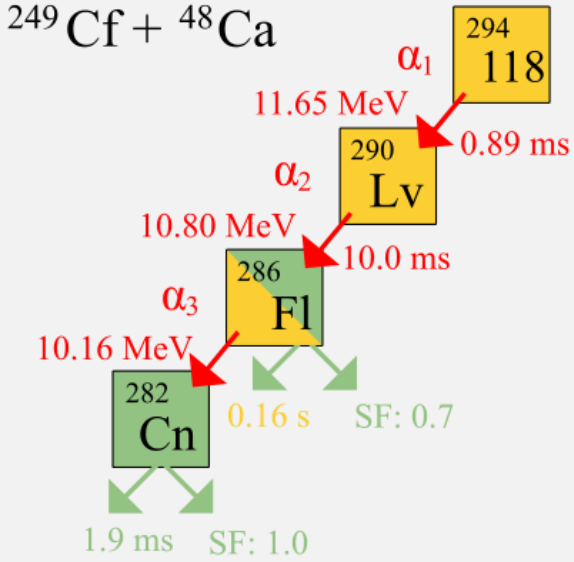
Search for new physics with atoms and molecules

M.S. Safronova, D. Budker, D. DeMille, Derek F. Jackson Kimball, A. Derevianko, and Charles W. Clark

Why investigate unstable and artificial elements?

- (Exotic) nuclear structure and properties
- Information about new elements, assignment in Periodic Table
- Behaviour and trends in lower part of the Periodic Table
- Benchmarks for theory (e.g. contribution of QED effects)
-





Challenging experiments!

- In one case, unprecedented sensitivity needed to detect the tiny effects of new physics
- In the other, dealing with small amounts of unstable, short lived elements

- Sometimes, combined challenges (e.g. precision measurements on RaF and others)!

- Alongside specially developed experimental techniques, theoretical support becomes crucial

How can (atomic and molecular) theory be of use?

- Practical parameters for experiments (predictions of transition energies, laser-cooling schemes, etc.)
- Parameters for the interpretation of the results (HFS parameters for extraction of nuclear properties, coupling parameters for new physics phenomena, etc.)
- Identification of promising candidates for precision measurements
  - High sensitivity
  - Experimental considerations (stability, laser-coolability, etc.)

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For use in experiments:

- Reliable predictions based on high accuracy calculations
- Preference for *ab initio* methods (predictive power)
- Possibility of assigning uncertainties

Choice of computational method becomes important

COMPUTATIONAL METHODS

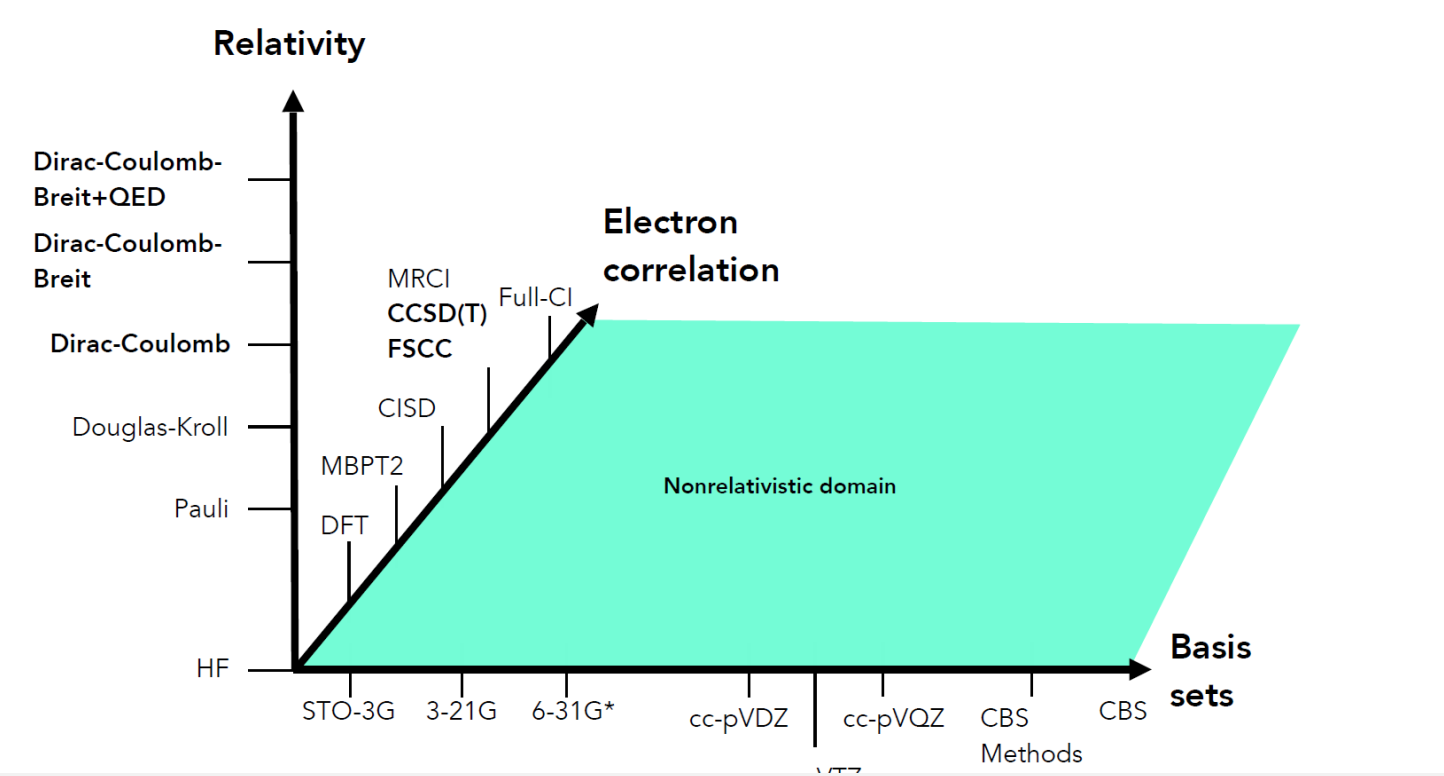
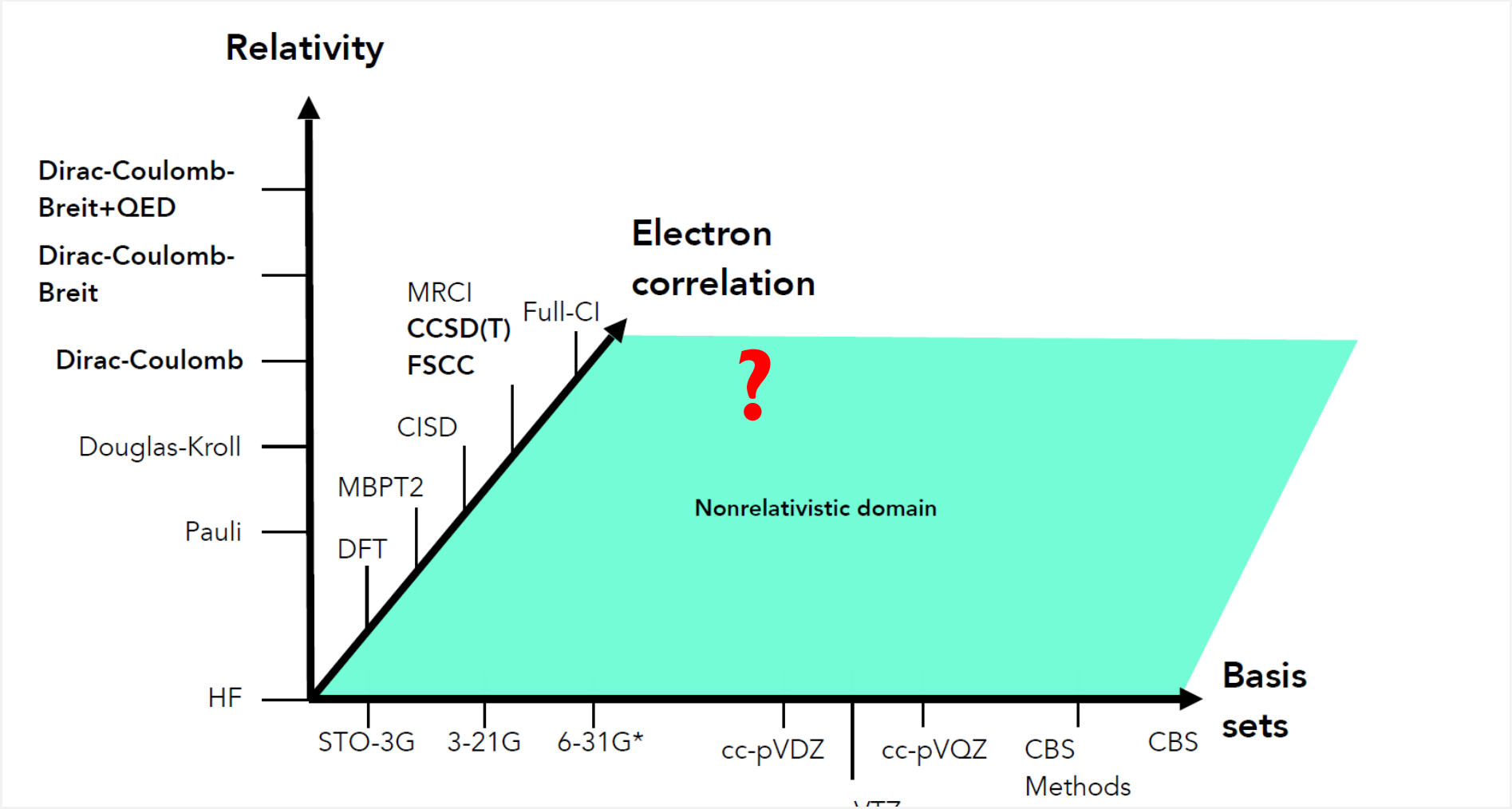


Figure courtesy of P. Schwerdtfeger


Relativity
Dirac-Coulomb-Breit+QED
Dirac-Coulomb-Breit
Dirac-Coulomb
Douglas-Kroll
Pauli
HF
Electron correlation
MRCI
CCSD(T)
FSCC
Full-CI
CISD
MBPT2
DFT
?
Nonrelativistic domain
Basis sets
STO-3G
3-21G
6-31G*
cc-pVDZ
cc-pVQZ
CBS
CBS Methods

What do we need?

- Coupling parameters describing the effect of *P*(*T*)-violating phenomena (or variation of constants) on electronic structure
  - Relativistic in nature, hence relativistic methods
- Atomic and molecular parameters needed in experiments
  - (usually) heavy (radioactive) systems, hence relativistic methods
- High accuracy
  - State-of-the-art treatment of correlation, large basis sets
- Uncertainty estimates
  - Robust, transparent methods

Relativistic coupled cluster

- Based on the 4c Dirac Hamiltonian
- Accurate, size-consistent

- **CCSD(T) -** single reference coupled cluster

Closed shell systems/systems with one dominant configuration (good example: BaF, $X\ ^2\Sigma$)

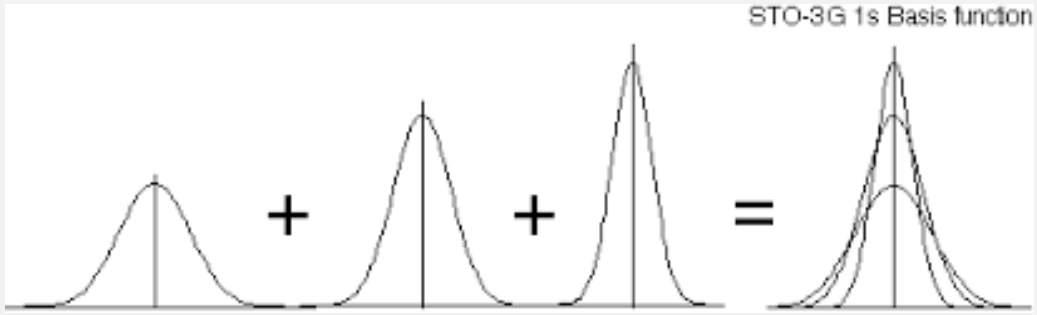
- **FSCC** – multireference Fock space coupled cluster

Open shell systems, excited states, bond dissociation (good example: ThO $^3\Delta_1$ or any atomic spectrum)

Use the suitable method, or both in complementary manner.

Basis sets

- Sets of (Gaussian) functions that are used to represent the electronic WF.
- Atom specific, different basis sets for different properties



$g = x^{\ell}\, y^{m}\, z^{n}\, e^{-\alpha r^2}$

'exponent' α

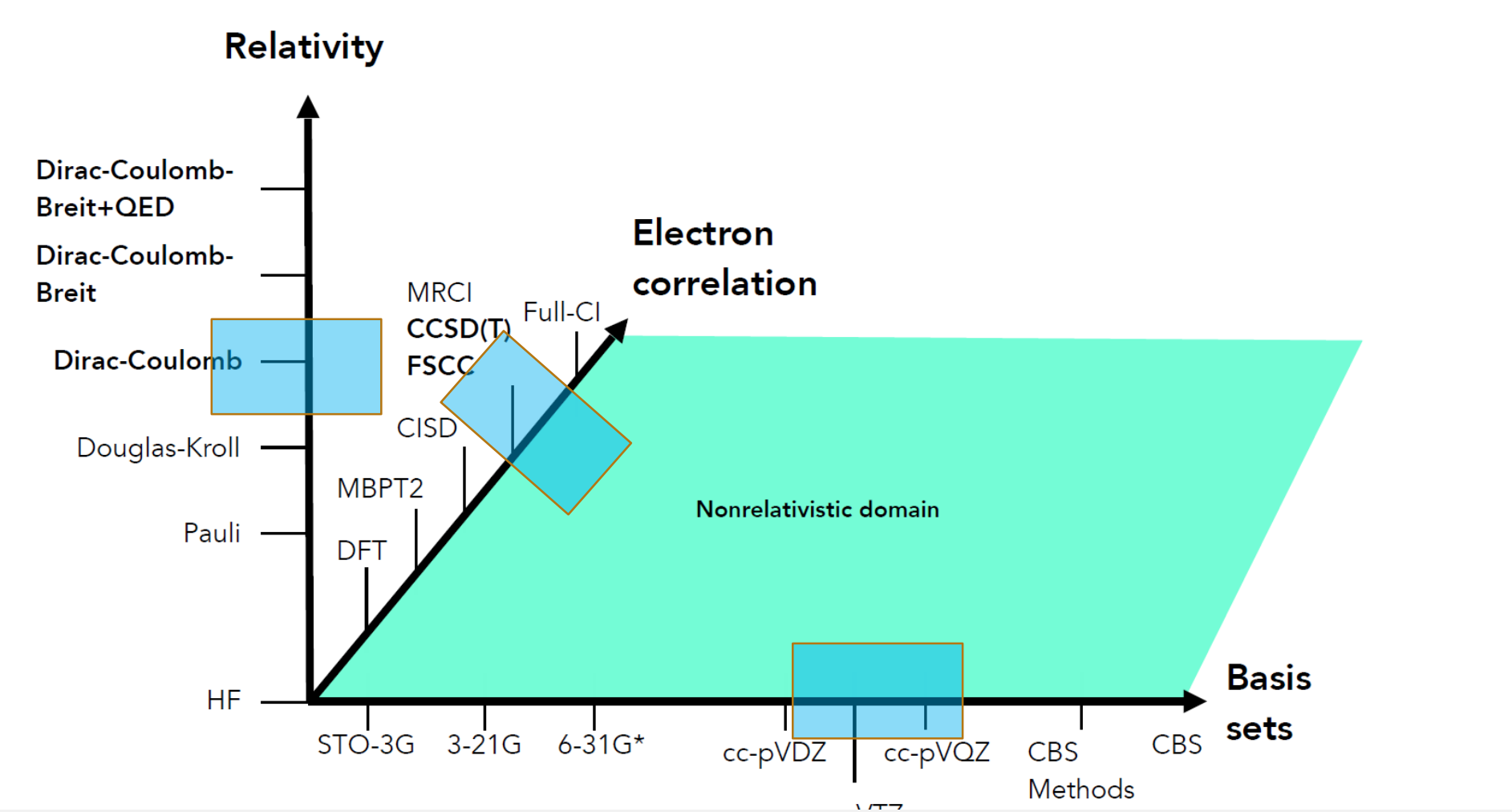
Gaussian type orbital

type of function:
$\ell = m = n = 0$ for s type
ℓ or m or n = 1 for p type
etc.

- Dyall's relativistic basis sets; augmented and extended to convergence

(K.G. Dyall, Theor. Chem Acc. 2002, 2004, 2006, 2007, 2009, 2011,2012, etc.)

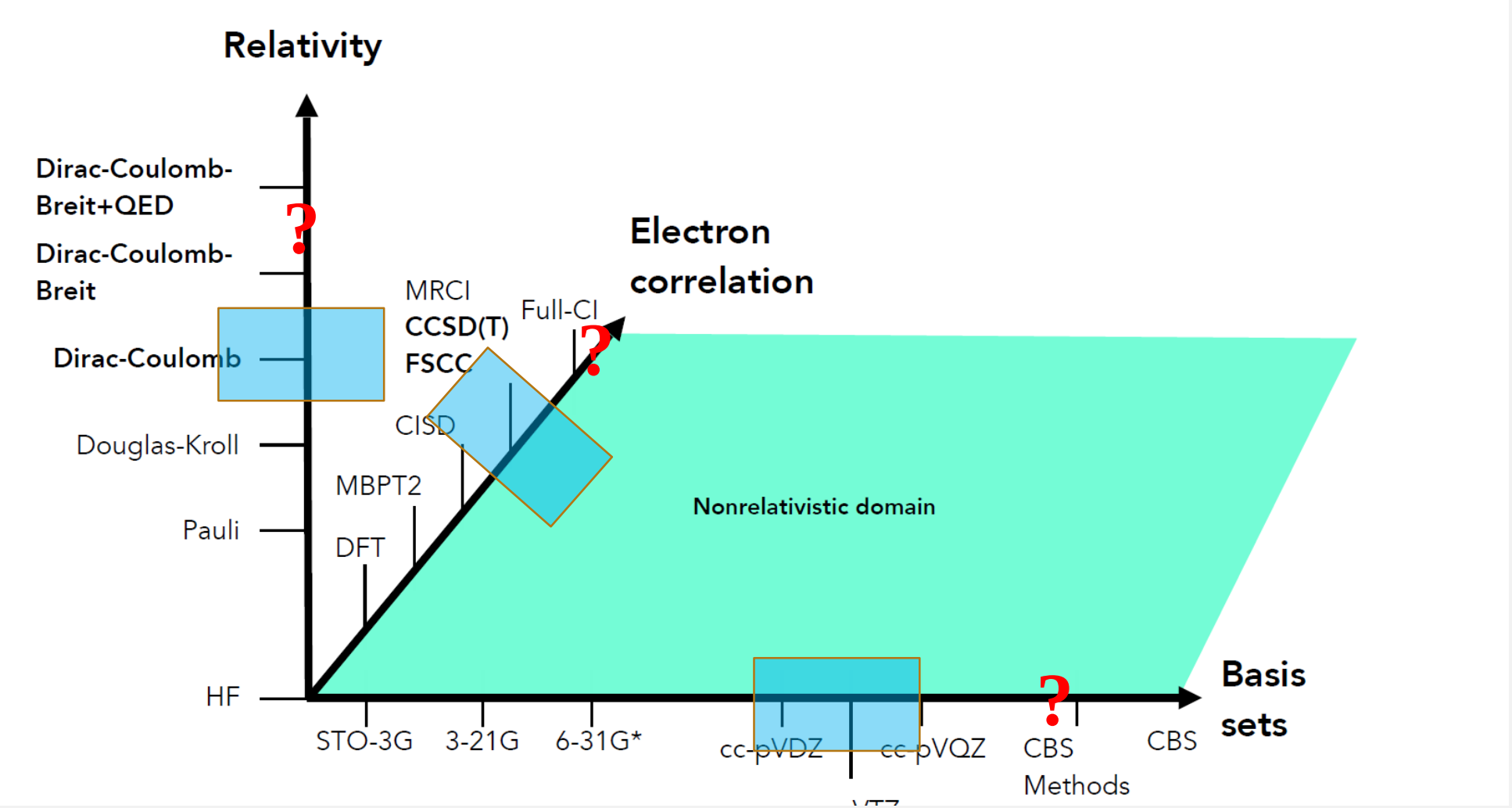
Relativistic coupled cluster



What can we calculate?

- Atomic properties: energies, IPs, EAs, spectra, hyperfine structure parameters, polarisabilities
- Molecular properties: geometries, spectroscopic constants, electronic structure, Franck-Condon Factors (FCFs), transition strengths
- Specific properties:
  - W_d, W_s (eEDM experiments)
  - W_A (NSD-PV, nuclear anapole moments)
  - W_M (nuclear magnetic quadrupole moments)
  - Sensitivity to variation of α
  - ...
- CCSD(T), FSCC (applicable to different systems/states)
- Expected accuracy: ~10 meV for energies, single % for properties
- Systematic investigation of effect of computational parameters and uncertainty evaluation

How do we assign uncertainties?



Software

- Tel Aviv atomic computational package (TRAFS-3C)

Tel-Aviv Relativistic Atomic Fock-Space coupled cluster code, written by E.Eliav and U.Kaldor, with contributions from Y. Ishikawa, A. Landau, A. Borschevsky and H. Yakobi.

- DIRAC18 computational package

DIRAC, a relativistic *ab initio* electronic structure program, release DIRAC18 (2018)

and:

- MRCC code of Kallay et al., www.mrcc.hu (higher excitations)
- CFOUR package, http://www.cfour.de (geometry optimisation of polyatomic molecules)

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Any drawbacks?

- ✗ Computationally expensive
- ✗ FSCC is limited to systems with up to two valence electrons/holes
- ✗ Some properties not (yet) available, e.g. TDMs

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Towards High Performance Relativistic Electronic Structure Modelling: The EXP-T Program Package

Alexander V. Oleynichenko, Andréi Zaitsevskii & Ephraim Eliav

APPLICATIONS

- Hyperfine structure constants:
  - New implementation and test cases
  - Ge
- Nuclear-spin-dependent parity violation measurements:
  - BaF
  - Light triatomic molecules

HYPERFINE STRUCTURE CONSTANTS

New implementation: magnetic hyperfine coupling constants

- Expectation values are difficult in CC: use finite field approach

$$\hat{H} = \hat{H}^{(0)} + \lambda \hat{H}^{\mathrm{HFS}}_{M,u}$$

$$A_{M,uv} = \frac{g_M}{\Omega} \left. \frac{\partial E_u^{\Omega_v}(\lambda)}{\partial \lambda} \right|_{\lambda=0}$$

$$\begin{aligned} \hat{H}^{M,\mathrm{HFS}} &= g_M \mu_N \vec{I}^M \cdot \sum_i \frac{(\vec{r}_{iM} \times \vec{\boldsymbol{\alpha}}_i)}{r_{iM}^3} \\ &= \sum_u g_M \mu_N I_u^M \sum_i \frac{(\vec{r}_{iM} \times \vec{\boldsymbol{\alpha}}_i)_u}{r_{iM}^3} \\ &= \sum_u I_u^M \hat{H}_u^{M,\mathrm{HFS}}. \end{aligned}$$

- Complementary with already existing implementation for electric quadrupole HFS constants
- Both single reference CCSD(T) and FSCC
- Applicable to atoms and molecules, ground and excited states

Ground states: Cs and BaF

- CCSD/CCSD(T) level of theory
- Uncertainty evaluation:

How do we assign uncertainties?

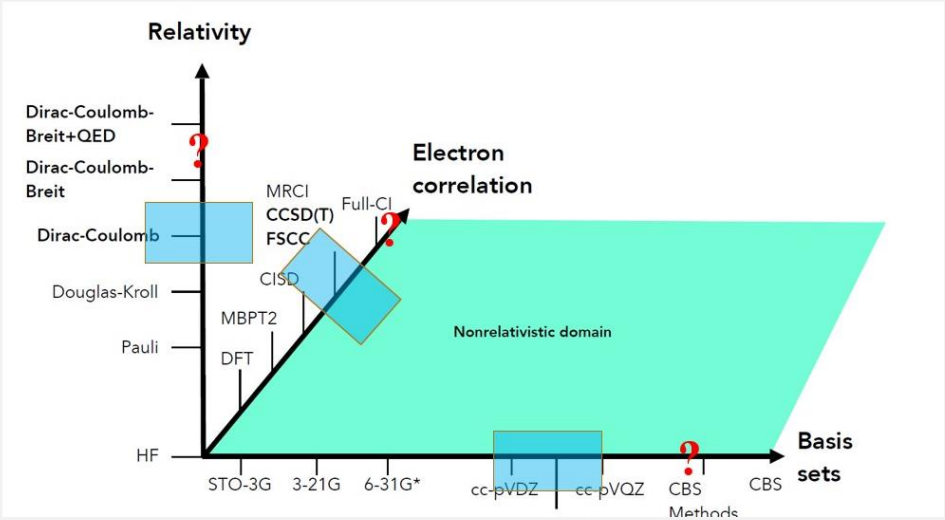
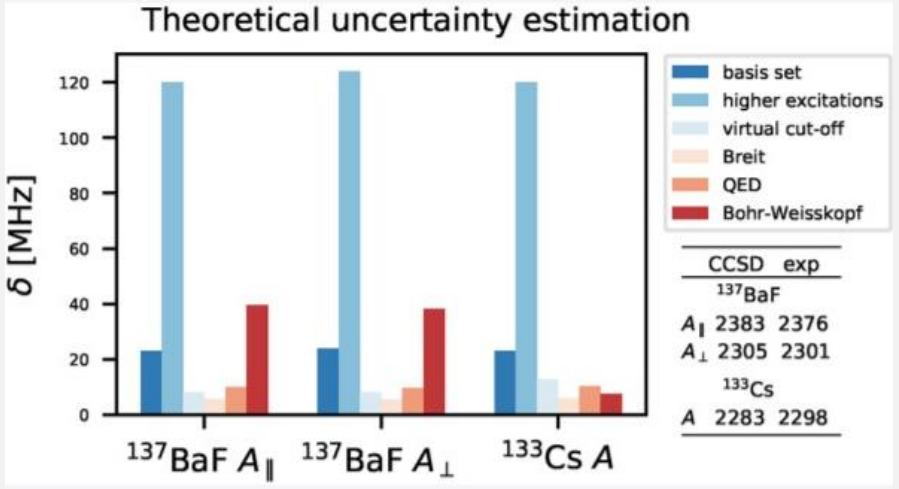


Table 7. Summary of the Sources of Uncertainty (MHz) of the Calculated $A_{\|}$, $A_{\perp}$, and A Constants (MHz) of ^{137}Ba in BaF and ^{133}Cs

source	^{137}BaF		^{133}Cs
	$\delta A_{\|}$	$\delta A_{\perp}$	δA
basis set			
quality	20.00	20.00	19.0
tight functions	3.00	3.00	4.00
diffuse functions	0.00	1.00	0.00
correlation			
higher order	−120.00	−124.00	−120.00
virtual cutoff	8.18	8.18[c]	12.78
relativistic effects			
Breit	5.72[a]	5.53[a]	6.00[b]
QED^{VP+SE}	−10.01[a]	−9.68[a]	−10.30[b]
Bohr−Weisskopf	−39.56[a]	−38.26[a]	−7.60[b]
quadratic sum	128.74	132.07	123.05
%	5.40	5.73	5.28

[a]Based on ^{135}Ba^{+} results from ref 85. [b]Taken directly from ref 85. [c]Used $A_{\|}$ results.



Ground states: Cs and BaF

Table 9. *A* of Cs in MHz[a]

method	^{133}Cs	%(exp)
MBPT[b]+B[7]	2291.00	−0.31
SDpT+B[8]	2278.5	−0.85
MBPT[b7]+B[10]	2295.87	−0.10
MBPT[b]+OE+G[9]	2302	0.17
CCSDvT[11]+B[10]+QED[VP+SE 87]	2306.6	0.36
CCSD (ECC)[26]	2179.1	−5.18
CCSD (Z-vector)[27]	2218.4	−3.47
MBPT[b]+B+QED[VP+SE 85]	2294.4	−0.16
CCSD (LCCSD)[81]	2345.9	2.08
CCSD (finite field, this work)	2283(123)	−0.66
exp[78]	2298.16	

Table 8. $A_\parallel$ and $A_\perp$ of ^{137}Ba in BaF (MHz)

	^{137}BaF			
method	$A_\parallel$	%(exp)	$A_\perp$	%(exp)
GRECP SCF-EO[90]	2264	−4.71	2186	−5.00
GRECP RASSCF-EO[90]	2272	−4.38	2200	−4.39
DF RASCI[91]	2240	−5.72	2144	−6.82
DF MBPT[91]	2314	−2.61	2254	−2.04
DC CCSD (this work)	2383(129)	0.29	2305(132)	0.17
exp[77]	2376(12)		2301(9)	

Ground states: Cs and BaF

Pi Haase

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THE JOURNAL OF PHYSICAL CHEMISTRY A

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Hyperfine Structure Constants on the Relativistic Coupled Cluster Level with Associated Uncertainties

Pi A. B. Haase,* Ephraim Eliav, Miroslav Iliaš, and Anastasia Borschevsky

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in BaF (MHz)

		^{137}BaF		
		%(exp)	$A_\perp$	%(exp)
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		−4.38	2200	−4.39
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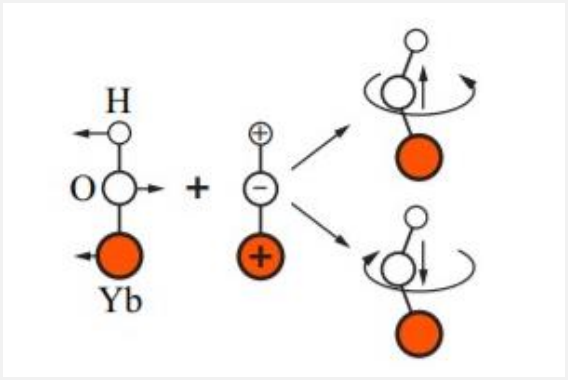
exp[77]	2376(12)		2301(9)	

Predictive power

- YbOH: promising candidate for search for eEDM and other P,T-violating effects.

TABLE VII. The $A_{\|}$ constants of the heavy nucleus calculated using the model optimized for W_M given in (MHz) and comparison with the available experimental data.

System	Calculated $A_{\|}$	Expt. $A_{\|}$	Δ (%)
^{137}BaOH	2194.6	2200.2[42]	0.3
^{171}YbF	7579.0	7429.1[43]	2
^{173}YbF	−2087.6	−2060.0[44]	1.3
^{171}YbOH	7174.9		
^{173}YbOH	−1976.3		



Malika Denis

Enhanced $\mathcal{P}, \mathcal{T}$-violating nuclear magnetic quadrupole moment effects in laser-coolable molecules

Cite as: J. Chem. Phys. **152**, 084303 (2020); https://doi.org/10.1063/1.5141065
Submitted: 03 December 2019 . Accepted: 06 February 2020 . Published Online: 25 February 2020

Malika Denis, Yongliang Hao, Ephraim Eliav, Nicholas R. Hutzler, Malaya K. Nayak, Rob G. E. Timmermans, and Anastasia Borschesvky

Fine and hyperfine interactions in ^{171}YbOH and ^{173}YbOH

J. Chem. Phys. **154**, 244309 (2021); https://doi.org/10.1063/5.0055293

Nickolas H. Pilgram[1], Arian Jadbabaie[1], Yi Zeng[1], Nicholas R. Hutzler[1], *and* Timothy C. Steimle[2,a)]

Table II: Comparison of the measured hyperfine parameters of the $\tilde{X}^2\Sigma^+(0,0,0)$ state of ^{171,173}YbOH to calculated values

Isotopologue	Parameter	Measured (MHz)	Theory Ref. [16] (MHz)	Theory Ref. [51] cGHF(MHz)	Theory Ref. [51] cGKS(MHz)	Theory Ref.[52] (MHz)
^{171}YbOH	$A_{\|\|}$ [a]	6979 (35)	7174.9			
^{171}YbOH	$A_{\perp}$ [b]	6745(15)				
^{173}YbOH	$A_{\|\|}$	-1929(11)	−1976.3	-1600	-1300	
^{173}YbOH	$A_{\perp}$	-1856 (5)		-1600		
^{173}YbOH	e^2Qq_0	-3319 (48)	−3502			-3492

TABL
optim
data.
Syst
^{137}B
^{171}Y
^{173}Y
^{171}Y
^{173}YbOH −1976.3

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Excited states: Ge

- Collinear laser spectroscopy performed at ISOLDE-CERN
- HFS of the $4s^2 4p^2\ {}^3\mathrm{P}_1 \rightarrow 4s^2 4p 5p\ {}^3\mathrm{P}_1{}^{o}$ transition
- ^{69,71,73}Ge
- Atomic calculations of A_0 and q (EFG) parameters used for analysis
- FSCC approach, uncertainty estimation

Configuration	Term	J	Level (cm^{-1})	Ref.
$4s^2 4p^2$	^{3}P	0	0.0000	SM93b
		1	557.1341	SM93b
		2	1409.9609	SM93b
$4s^2 4p^2$	^{1}D	2	7125.2989	SM93b
$4s^2 4p^2$	^{1}S	0	16367.3332	SM93b
$4s^2 4p5s$	^{3}P°	0	37451.6893	SM93b
		1	37702.3054	SM93b
		2	39117.9021	SM93b

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$4s^2 4p5s$	$^3P^\circ$	0	37451.6893	SM93b
		1	37702.3054	SM93b
		2	39117.9021	SM93b

Electric field gradient uncertainties — Germanium

	$4p^2\ ^3P_1$	$4p^2\ ^3P_2$	$4p5s\ ^3P_1$
Basis set	0.0043	0.0078	0.0488
Model space	0.0007	0.0016	0.0103
Virtual space	0.0003	0.0004	0.0001
Triples+higher	0.0353	0.0720	0.0266
Gaunt	0.0001	0.0051	0.0016
Total uncertainty	3.0 %	3.0 %	6.4 %
q^{th} (a.u.)	**1.178(36)**	**-2.399(73)**	**-0.885(56)**

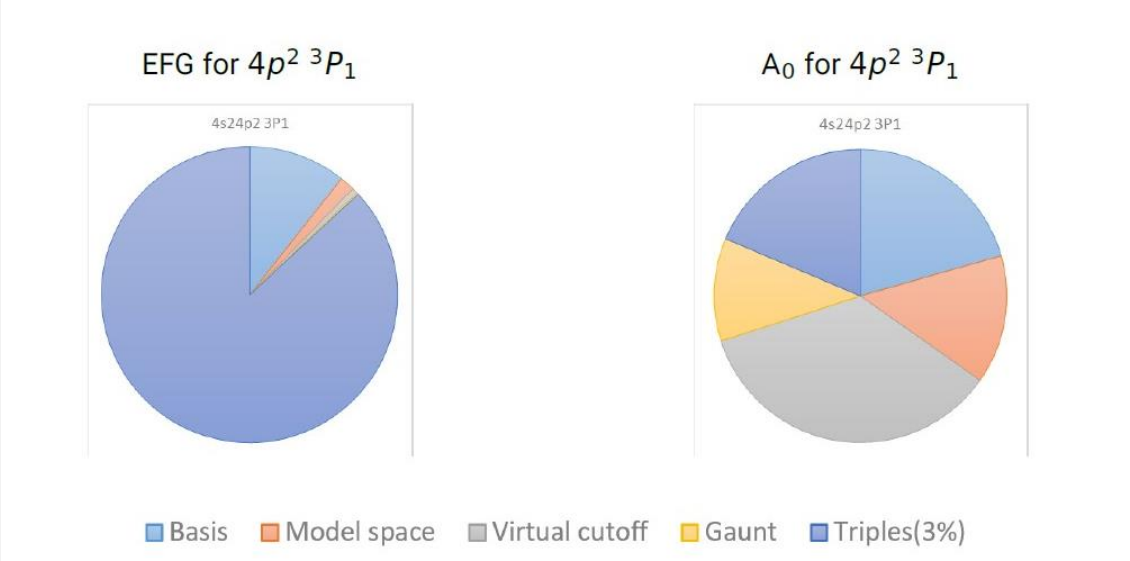
Table: Sources of uncertainty and final values of the calculated q^{th} (a.u.).

A_0 uncertainties — Germanium

	$4p^2\ ^3P_1$	$4p^2\ ^3P_2$	$4p5s\ ^3P_1$
Basis set	2.5	4.3	18.1
Model space	1.7	2.7	9.0
Virtual space	4.2	3.1	4.6
Triple+higher	2.2	9.6	39.4
Gaunt	1.4	0.4	2.7
Total uncertainty	7.8 %	3.5 %	3.4 %
A_0^{th} (MHz)	**-74(6)**	**321(11)**	**1314(45)**

Table: Sources of uncertainty and final values of the calculated A_0^{th} (MHz).

Excited states: Ge (uncertainties)



- Uncertainties should be evaluated separately for different states and properties.

Ge moments

	I^π	$\mu^{lit}(\mu_N)$	$\mu^{exp}(\mu_N)$
^{69}Ge	$5/2^-$	+0.735(7) [1]	+0.920(5)
^{71}Ge	$1/2^-$	+0.54606(7) [2]	+0.547(5)
^{73}Ge	$9/2^+$	-0.87824(5) [3]	-0.904(21)

	I^π	$Q_s^{lit}(b)$	$Q_s^{exp}(b)$	$Q_s^{JUN45}(b)$
^{69}Ge	$5/2^-$	+0.027(5) [1]	+0.114(7)	+0.150
^{73}Ge	$9/2^+$	-0.196(1) [4]	-0.198(4)	-0.258

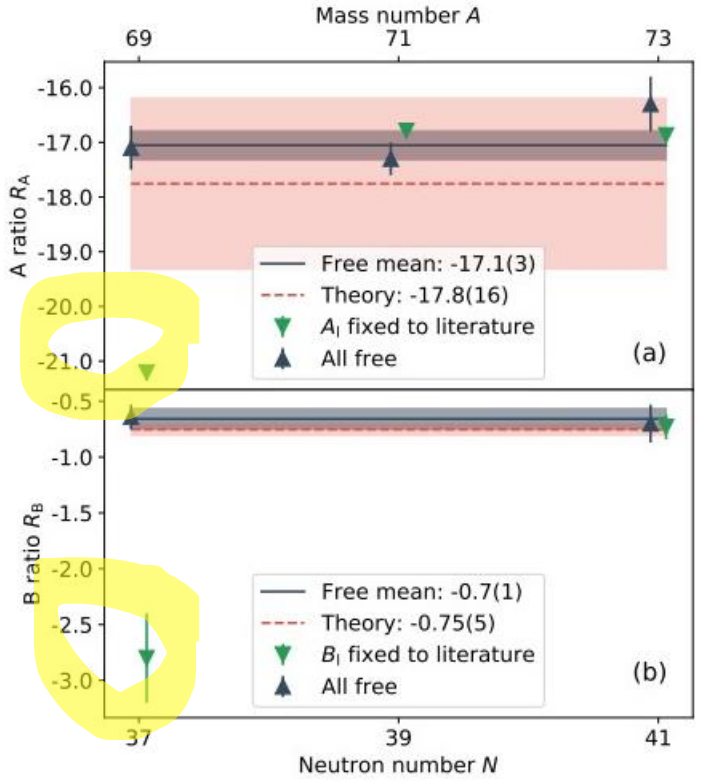


FIG. 4. Ratio of the A (a) and B hyperfine constants (b) for the $4p^2\,{}^3P_1$ (lower) and $4p5s\,{}^3P_1^o$ (upper) atomic states, deduced with two fitting procedures. One with the A_I and B_I values for each isotope fixed (green) to the high-precision value reported in literature [24, 28, 36], and one with all hyperfine constants as free fit parameters (black). The hyperfine constants ratios calculated with atomic relativistic FSCC are shown by red dashed lines.

[1] A. F. Oluwole, S. G. Schmelling, and H. A. Shugart, Phys. Rev. C 2, 228 (1970).
[2] W. J. Childs and L. S. Goodman, Phys. Rev. 141, 15 (1966).
[3] W. Makulski, K. Jackowski, A. Antušek, and M. Jaszunski, J. Phys. Chem. A 110, 11462 (2006).
[4] V. Kellö and A. Sadlej, Mol. Phys. 96, 275 (1999).

Ge moments

Martijn Reitsma

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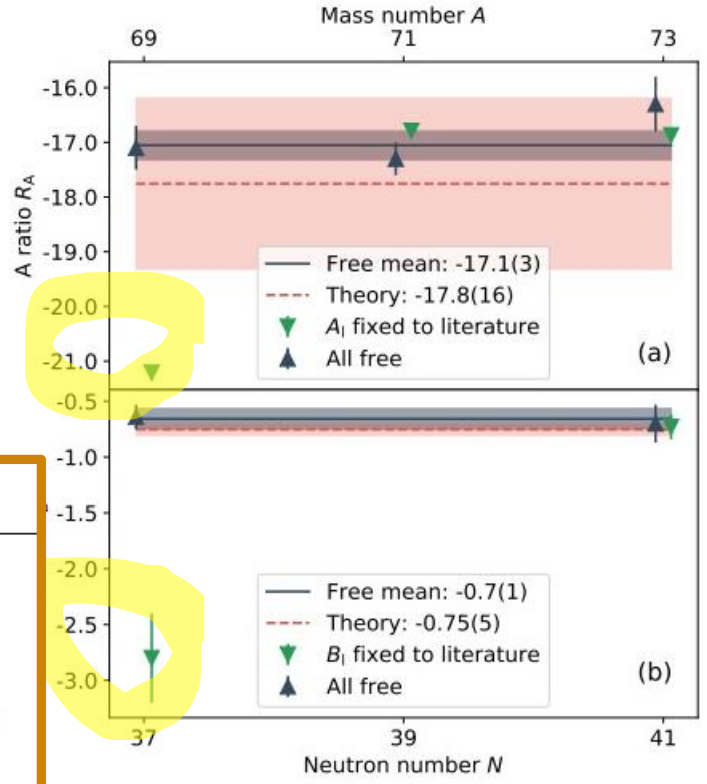
^{73}Ge				

PHYSICAL REVIEW C **102**, 054331 (2020)

Nuclear moments of germanium isotopes near $N = 40$

A. Kanellakopoulos,[1] X. F. Yang,[2,1,*] M. L. Bissell,[3] M. L. Reitsma,[4] S. W. Bai,[2] J. Billowes,[3] K. Blaum,[5] A. Borschevsky,[4] B. Cheal,[6] C. S. Devlin,[6] R. F. Garcia Ruiz,[7,†] H. Heylen,[7] S. Kaufmann,[8,9] K. König,[8,‡] Á. Koszorús,[1,§] S. Lechner,[7,10] S. Malbrunot-Ettenauer,[7] R. Neugart,[5,9] G. Neyens,[1,7] W. Nörtershäuser,[8] T. Ratajczyk,[8] L. V. Rodríguez,[5,11,‖] S. Sels,[7,¶] S. J. Wang,[2] L. Xie,[3] Z. Y. Xu,[1,#] and D. T. Yordanov[11]

^{69}Ge	$5/2^-$	+0.027(5) [1]	+0.114(7)	+0.150
^{73}Ge	$9/2^+$	-0.196(1) [4]	-0.198(4)	-0.258



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[4] V. Kellö and A. Sadlej, Mol. Phys. 96, 275 (1999).

NUCLEAR SPIN DEPENDENT PV EFFECTS

Search for new physics with atoms and molecules

M. S. Safronova, D. Budker, D. DeMille, Derek F. Jackson Kimball, A. Derevianko, and Charles W. Clark
Rev. Mod. Phys. **90**, 025008 – Published 29 June 2018

Anapole moment measurement in BaF

- NSD PV effects in atoms/molecules:

$$H_{\mathrm{NSD}} = \frac{G_F}{\sqrt{2}I} \sum_i (\kappa_A + \kappa_{\mathrm{ax}} + \kappa_{\mathrm{hfs}}) (\boldsymbol{\alpha}_i \cdot \boldsymbol{I}) \rho(\boldsymbol{r}_i)$$

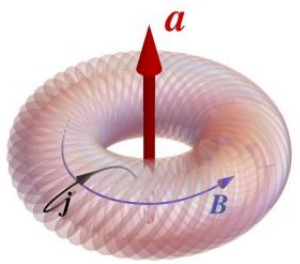

FIG. 7 (Color online) The toroidal component of current density $\boldsymbol{j}$ produces anapole moment $\boldsymbol{a}$, with magnetic field $\boldsymbol{B}$ that is entirely confined inside the "doughnut". The azimuthal component of current density generates magnetic dipole moment aligned with $\boldsymbol{a}$, with its associated conventional dipolar magnetic field not shown.

- Nuclear anapole moment is the dominant NSD-PV effect in heavy systems
- Measurement can provide stringent test of SM and nuclear theory
- Planned measurement on BaF*
- W_A coefficient can be used to extract anapole from measurements

$$W_A = \frac{G_F}{\sqrt{2}} \left\langle +\tfrac{1}{2} \right| \sum_i \rho(\boldsymbol{r}_i) \alpha_+ \left| -\tfrac{1}{2} \right\rangle .$$

$$\alpha_+ = \alpha_x + i\alpha_y = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + i \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}$$

*E. Altuntas et al., PRL **120**, 142501 (2018)

Anapole moment measurement in BaF

Method	W_A (Hz)	Ref.
CCSD(T)+Gaunt	**147.7±2**	**Present**
RECP+SCF+EO	181	Kozlov et al., PRA **56** R3326 (1997)
Semiempirical	164	DeMille et al., PRL **100**, 023003 (2008)
4c-RASCI	160	Nayak and Das, PRA **79**, 060502 (2009)
Scaled ZORA-HF	190	Isaev & Berger, PRA **86**, 062515 (2012)
DHF/DFT+CP	146	Borschevsky et al., PRA **88**, 022125 (2013)

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- Quick sanity check:

Table 8. $A_\parallel$ and $A_\perp$ of ^{137}Ba in BaF (MHz)

	^{137}BaF			
method	$A_\parallel$	%(exp)	$A_\perp$	%(exp)
GRECP SCF-EO[90]	2264	−4.71	2186	−5.00
GRECP RASSCF-EO[90]	2272	−4.38	2200	−4.39
DF RASCI[91]	2240	−5.72	2144	−6.82
DF MBPT[91]	2314	−2.61	2254	−2.04
DC CCSD (this work)	2383(129)	0.29	2305(132)	0.17
exp[77]	2376(12)		2301(9)	

Anapole moment measurement in BaF

Method	W_A (Hz)	Ref.
CCSD(T)+Gaunt	**147.7±2**	**Present**
RECP+SCF+EO	181	Kozlov et al., PRA **56** R3326 (1997)
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Scal		
DH		

Yongliang Hao

- Qu

PHYSICAL REVIEW A **98**, 032510 (2018)

Nuclear anapole moment interaction in BaF from relativistic coupled-cluster theory

Yongliang Hao,[1] Miroslav Iliaš,[2] Ephraim Eliav,[3] Peter Schwerdtfeger,[4,5] Victor V. Flambaum,[6,7] and Anastasia Borschevsky[1,*]

GRECP SCF-EO[90]	2264	−4.71	2186	−5.00
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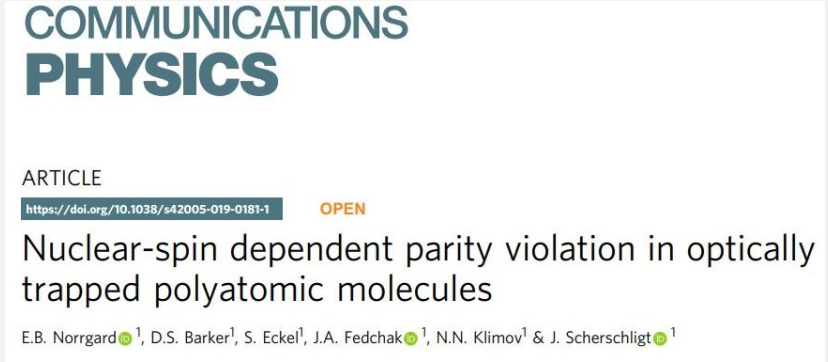
exp[77]	2376(12)		2301(9)	

NSD-PV effects in light polyatomic molecules

- NSD PV effects in atoms/molecules:

$$H_{\mathrm{NSD}} = \frac{G_F}{\sqrt{2}I} \sum_i (\kappa_A + \kappa_{\mathrm{ax}} + \kappa_{\mathrm{hfs}}) (\boldsymbol{\alpha}_i \cdot \boldsymbol{I}) \rho(\boldsymbol{r}_i)$$

- In light systems these contributions are similar in size
- Measurement can provide stringent tests of SM, nuclear theory, probe the *Z*-boson exchange between the electrons and the nuclei, and offer the possibility to search for new particles, such as the *Z'* boson
- Measurements planned on BeNC, BeCN, MgNC, and MgCN
- Presence of different atoms: possibility to disentangle the contributions



NSD-PV effects in light polyatomic molecules

- In light system accurate nuclear theory predictions tangible:

- Together with predicted molecular enhancement factors can be used to estimate the expected measurable effect.

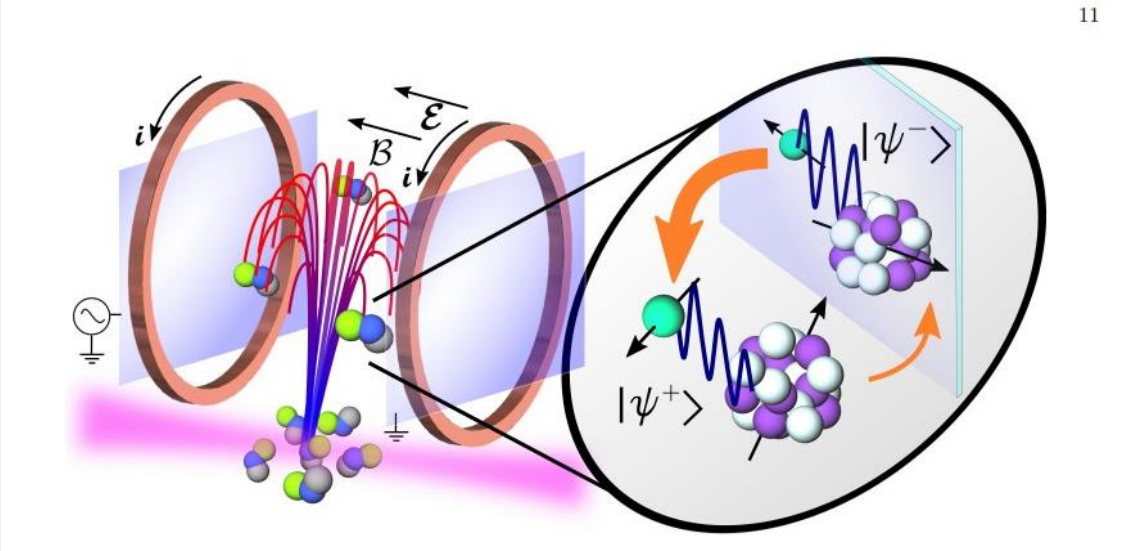


TABLE I: Magnetic moments (in units of nuclear magneton) [28, 61–65], anapole-moment coupling constants, spin operator matrix elements, and κ_{ax} coupling constants for ^{9}Be, ^{13}C, ^{14,15}N and ^{25}Mg obtained within NCSM. The results obtained using the single-particle model are also shown, along with the valence particle (V.p.) and the valence orbital (V.o) for each nucleus.

	^{9}Be	^{13}C	^{14}N	^{15}N	^{25}Mg
I^π	$3/2^-$	$1/2^-$	1^+	$1/2^-$	$5/2^+$
$\mu^{\text{exp.}}$	-1.177[a]	0.702[b]	0.404[c]	-0.283[d]	-0.855[e]
	NCSM calculations				
μ	-1.05	0.44	0.37	-0.25	-0.50
κ_A	0.016	-0.028	0.036	0.088	0.035
$\langle s_{p,z}\rangle$	0.009	-0.049	-0.183	-0.148	0.06
$\langle s_{n,z}\rangle$	0.360	-0.141	-0.1815	0.004	0.30
κ_{ax}	0.035	-0.019	0.0002	0.015	0.024
κ	0.050	-0.046	0.037	0.103	0.057
	Single-particle model calculations				
V. p.	n	n	n, p	p	n
V. o.	$p_{3/2}$	$p_{1/2}$	$p_{1/2}$	$p_{1/2}$	$d_{5/2}$
K	-2	1	1	1	-3
κ_A	0.007	-0.007	0.035	0.044	0.014
κ_{ax}	0.050	-0.017	0.0	0.017	0.050
κ_{hfs}	-0.001	0.001	0.0006	-0.0004	-0.002
κ	0.056	-0.023	0.036	0.060	0.062

TABLE V: Recommended values of the W_{PV} parameters (Hz) with corresponding uncertainties.

Mol. \ Atom	Atom 1		Atom 2	Atom 3
	Be	Mg		
BeNC	0.50	–	0.34	0.004
BeCN	0.54	–	0.28	0.030
MgNC	–	5.3	0.45	0.014
MgNC†	–	5.3	0.47	0.014
MgCN	–	5.4	0.37	0.064
Uncertainty (%)	6.3	4.9	7.6	8.2

NSD-PV effects in light polyatomic molecules

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TABLE I: Magnetic moments (in units of nuclear magneton) [28, 61–65], anapole-moment coupling constants, spin operator matrix elements, and κ_{ax} coupling constants for ^{9}Be, ^{13}C, ^{14,15}N and ^{25}Mg obtained within NCSM. The results obtained using the single-particle model are also shown, along with the valence particle (V.p.) and the valence orbital (V.o) for each nucleus.

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I^{π}	$3/2^{-}$	$1/2^{-}$	1^{+}	$1/2^{-}$	$5/2^{+}$
$\mu^{\text{exp.}}$	-1.177[a]	0.702[b]	0.404[c]	-0.283[d]	-0.855[e]
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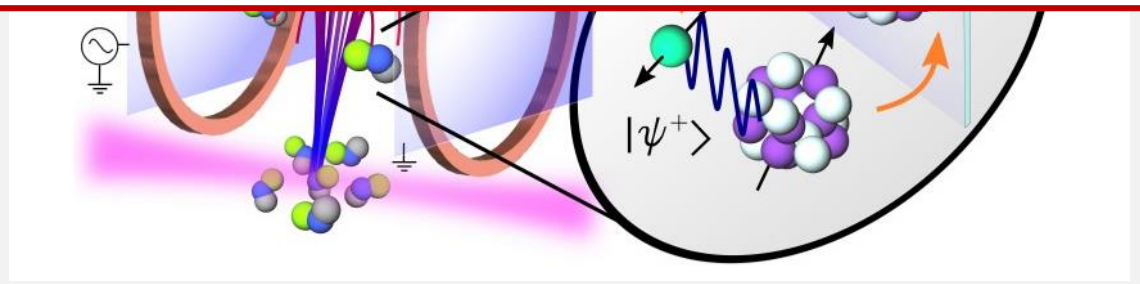
μ	-1.05	0.44	0.37	-0.25	-0.50
κ_{A}	0.016	-0.028	0.036	0.088	0.035
$\langle s_{p,z} \rangle$	0.009	-0.049	-0.183	-0.148	0.06
				15	0.004	0.30
				02	0.015	0.024
				7	0.103	0.057
				del calculations		
				p	n
				$p_{1/2}$	$d_{5/2}$
				1	-3
				5	0.044	0.014
					0.017	0.050
				06	-0.0004	-0.002
				6	0.060	0.062

Editors' Suggestion

Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao, Petr Navrátil, Eric B. Norrgard, Miroslav Iliaš, Ephraim Eliav, Rob G. E. Timmermans, Victor V. Flambaum, and Anastasia Borschevsky

Phys. Rev. A **102**, 052828 – Published 25 November 2020



l values of the W_{PV}
onding uncertainties.

Mol. \ Atom	Atom 1 Be	Atom 1 Mg	Atom 2	Atom 3
BeNC	0.50	–	0.34	0.004
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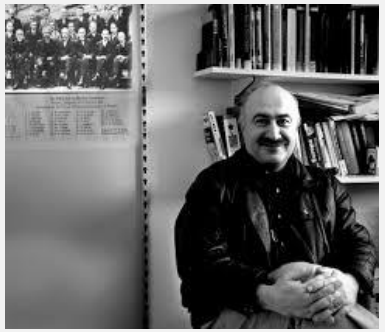
MgNC	–	5.3	0.45	0.014
MgNC†	–	5.3	0.47	0.014
MgCN	–	5.4	0.37	0.064
Uncertainty (%)	6.3	4.9	7.6	8.2

CONCLUSIONS

- State of the art high accuracy computational approach
- Versatile method: many possible applications
- Reliable predictions, uncertainty estimates possible
- Close collaborations with experimental groups

- These are very exciting times!

TEL AVIV UNIVERSITY
אוניברסיטת תל-אביב



Ephraim Eliav

Miroslav Ilias

Lukas Pasteka

UNSW
THE UNIVERSITY OF NEW SOUTH WALES
SYDNEY • AUSTRALIA

Victor Flambaum

Peter Schwerdtfeger

CTCP
Centre *for* Theoretical
Chemistry *and* Physics

RELATIVISTIC COUPLED CLUSTER

- Based on the 4c Dirac Hamiltonian
- Exponential wave operator:

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

- S is the excitation operator:

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

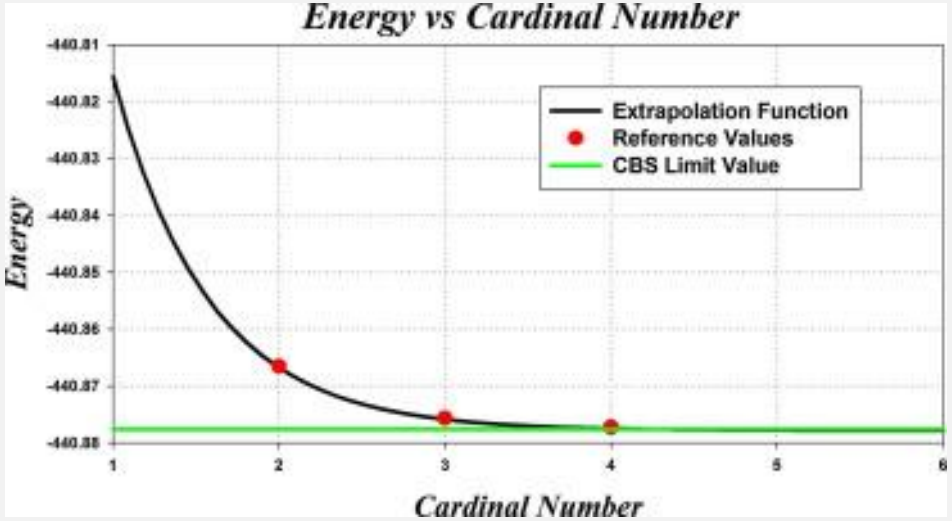
- CC energy equations:

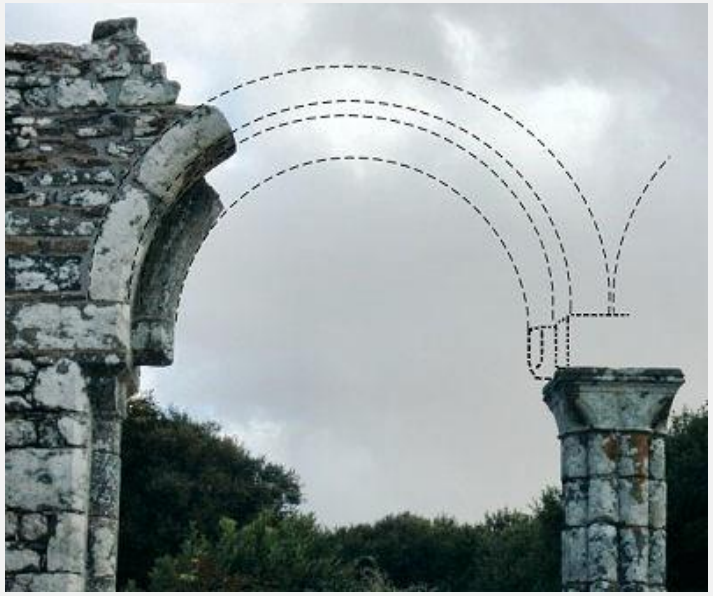
$$\langle \Phi_0 | (H - E_{\mathrm{CCSD}}) \exp(S_1 + S_2) | \Phi_0 \rangle = 0$$

- Accurate, all-order in PT, size-extensive, and size-consistent

Reaching meV accuracy

Complete basis set limit extrapolation





V. Vasilyev, http://sf.anu.edu.au/~vvv900/cbs