MOLECULES AS PROBES OF THE STANDARD MODEL AND ITS EXTENSIONS (THEORETICAL PERSPECTIVE)

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university of groningen
faculty of science and engineering
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- University of Groningen

<u>Research:</u>

Using state of the art methods from computational chemistry for high accuracy calculations of atomic and molecular properties in the context of 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

TALK OVERVIEW

- Motivation: why do we use molecules to test the Standard Model?
- Why do we need electronic structure theory?
- How do we perform accurate calculations and assign uncertainties?
- Applications

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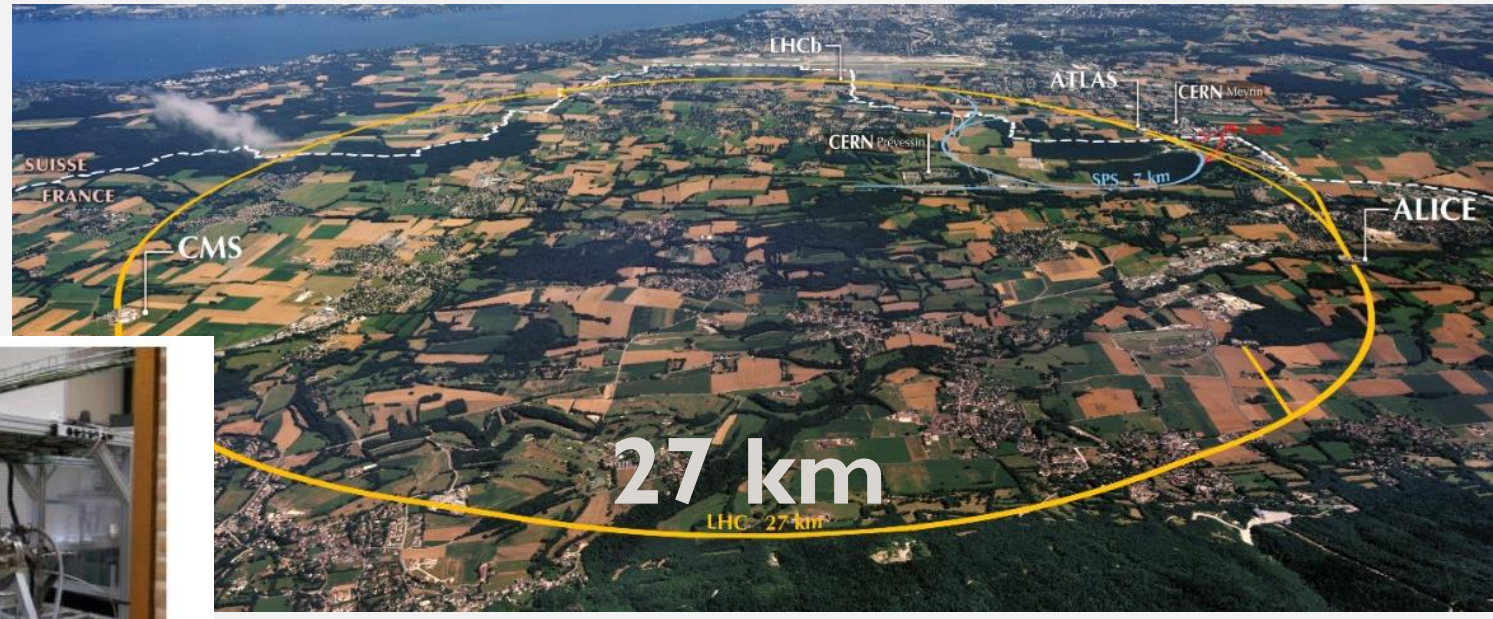
MOTIVATION

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

- Accelerator research (LHCb, 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 molecules?

- We are looking for truly tiny effects (signs of asymmetry)
- Electronic structure acts as an amplifier, bringing these effects into measurable range
- Example: electric dipole moment of the electron (eEDM)
  - Violates P,T – symmetry
  - Standard Model prediction: ~10^{-38} e·cm (too small for direct measurement)
  - Other theories predict lager values (still too small for direct measurement)
  - In a polar molecule, the internal electric field amplifies the electron EDM by 5 orders of magnitude→ we can try to measure it

Why look for physics beyond the SM with molecules?

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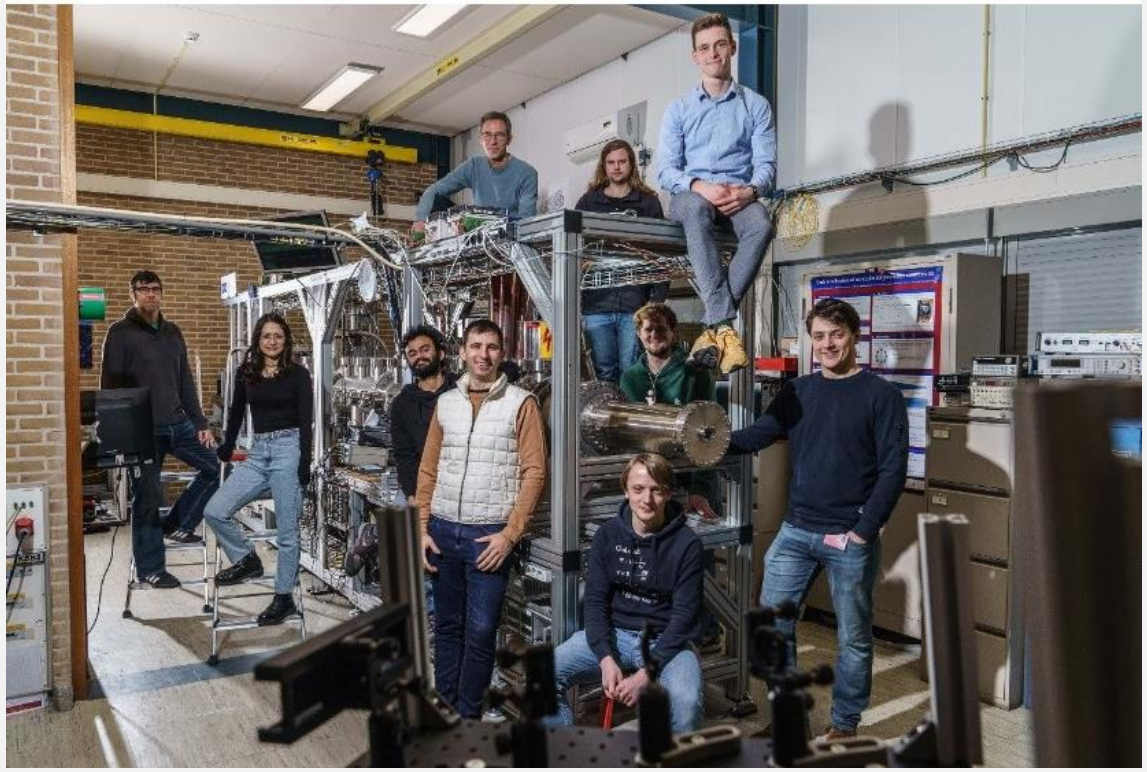
- Electronic structure acts as an amplifier, bringing these effects into measurable range
- For example: electric dipole moment of the electron (eEDM)
  - Similar for other P(T)-violating properties and BSM effects
  - Similar for parity violation

Why look for physics beyond the SM with molecules?

- **Table-top experiments with molecules: a 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



Why look for physics beyond the SM with radioactive molecules?

- Heavy systems, effects scale as Z^{2-5}
- Possible strong further enhancements due to the nuclear structure
- Sensitive to hadronic EDMs, nuclear magnetic quadrupole moments, etc.

Reports on Progress in **Physics**

REPORT ON PROGRESS

Opportunities for fundamental physics research with radioactive molecules

Gordon Arrowsmith-Kron, Michail Athanasakis-Kaklamanakis, Mia Au, Jochen Ballof, Robert Berger, Anastasia Borschevsky, Alexander A Breier, Fritz Buchinger, Dmitry Budker, Luke Caldwell, Christopher Charles, Nike Dattani, Ruben P de Groote, David DeMille, Timo Dickel, Jacek Dobaczewski, Christoph E Düllmann, Ephraim Eliav, Jonathan Engel, Mingyu Fan, Victor Flambaum, Kieran T Flanagan, Alyssa N Gaiser, Ronald F Garcia Ruiz, Konstantin Gaul, Thomas F Giesen, Jacinda S M Ginges, Alexander Gottberg, Gerald Gwinner, Reinhard Heinke, Steven Hoekstra, Jason D Holt, Nicholas R Hutzler, Andrew Jayich, Jonas Karthein, Kyle G Leach, Kirk W Madison, Stephan Malbrunot-Ettenauer, Takayuki Miyagi, Iain D Moore, Scott Moroch, Petr Navratil, Witold Nazarewicz, Gerda Neyens, Eric B Norrgard, Nicholas Nusgart, Lukáš F Pašteka, Alexander N Petrov, Wolfgang R Plaß, Roy A Ready, Moritz Pascal Reiter, Mikael Reponen, Sebastian Rothe, Marianna S Safronova, Christoph Scheidenerger, Andrea Shindler, Jaideep T Singh, Leonid V Skripnikov, Anatoly V Titov, Silviu-Marian Udrescu, Shane G Wilkins and Xiaofei Yang

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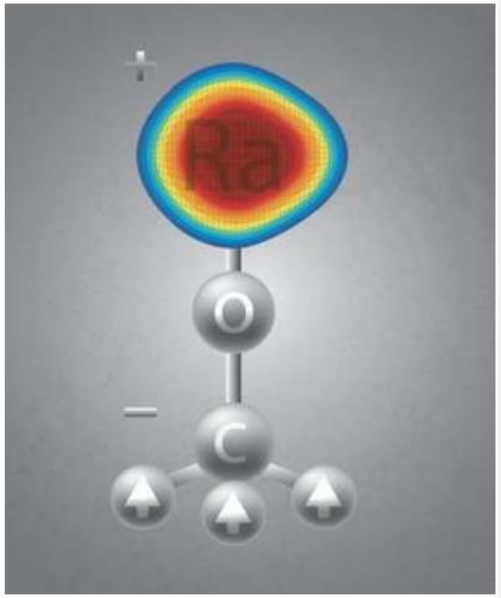
Reports on Progress in Physics, Volume 87, Number 8

Citation Gordon Arrowsmith-Kron *et al* 2024 *Rep. Prog. Phys.* **87** 084301

https://phys.org/news/2021-03-radioactive-molecules-mystery-antimatter.html



Promising yet challenging…

- Challenge of achieving unprecedented sensitivity needed to detect the tiny effects of new physics
- For radioactive systems, extra challenge of dealing with small amounts of short-lived atoms

- Alongside specially developed experimental techniques, theoretical support becomes crucial

TALK OVERVIEW

- Motivation: why do we use molecules to test the Standard Model?
- Why do we need electronic structure theory?
- How do we perform accurate calculations and assign uncertainties?
- Applications

How can (molecular) theory be of use?

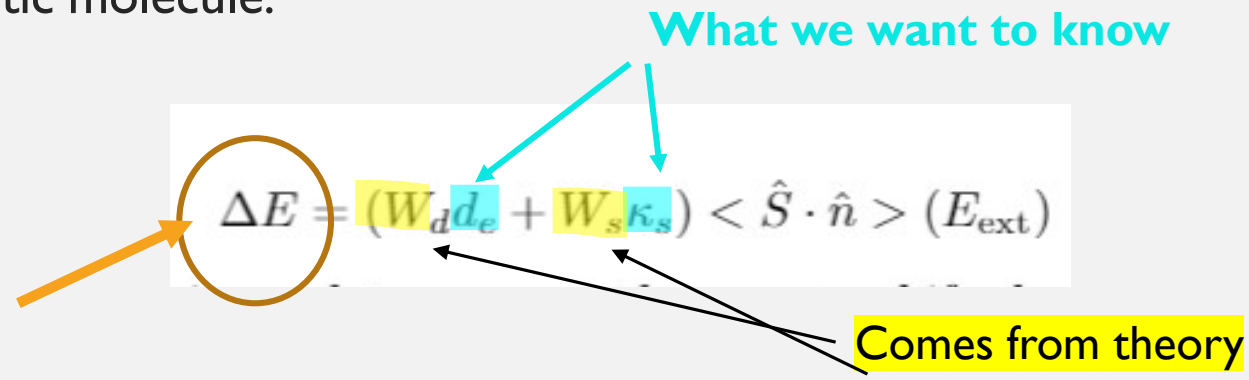
(Important to remember: for us the practical considerations do not play a role!)

- Insight into effect of new physics on molecular properties
- Identification of promising candidates for measurements
  - High sensitivity
  - Experimental considerations (stability, laser-coolability, etc.)
- Practical parameters for experiment (predictions of transition energies, laser-cooling schemes, etc.)
- Parameters for the interpretation of the results (coupling parameters for new physics phenomena, etc.)

How can (molecular) theory be of use?

(Important to remember: for us the practical considerations do not play a role!)

- Parameters for the interpretation of the results (coupling parameters for new physics phenomena, etc.)
- *P(T)*-violating energy (frequency) shift is obtained in experiment by reversing parity (reversing the direction of external fields): ΔE
- This energy difference can be related to the underlying *P*(*T*)-violating phenomena through electronic structure parameters (coupling constants)
- Example: P,T-violating effects in a paramagnetic molecule:



Theoretical predictions

For use in experiments, theoretical predictions should be

- Reliable
- Based on high accuracy calculations
- Be accompanied by uncertainties:
  - Important for planning the measurements (e.g. what range should be scanned?)
  - Important for extraction of properties of interest (uncertainty on the extracted new physics parameters will include the theoretical uncertainty)

Thus, we need an accurate method that allows uncertainty estimation!

TALK OVERVIEW

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COMPUTATIONAL METHODS

We would like to solve the Schroedinger equation.

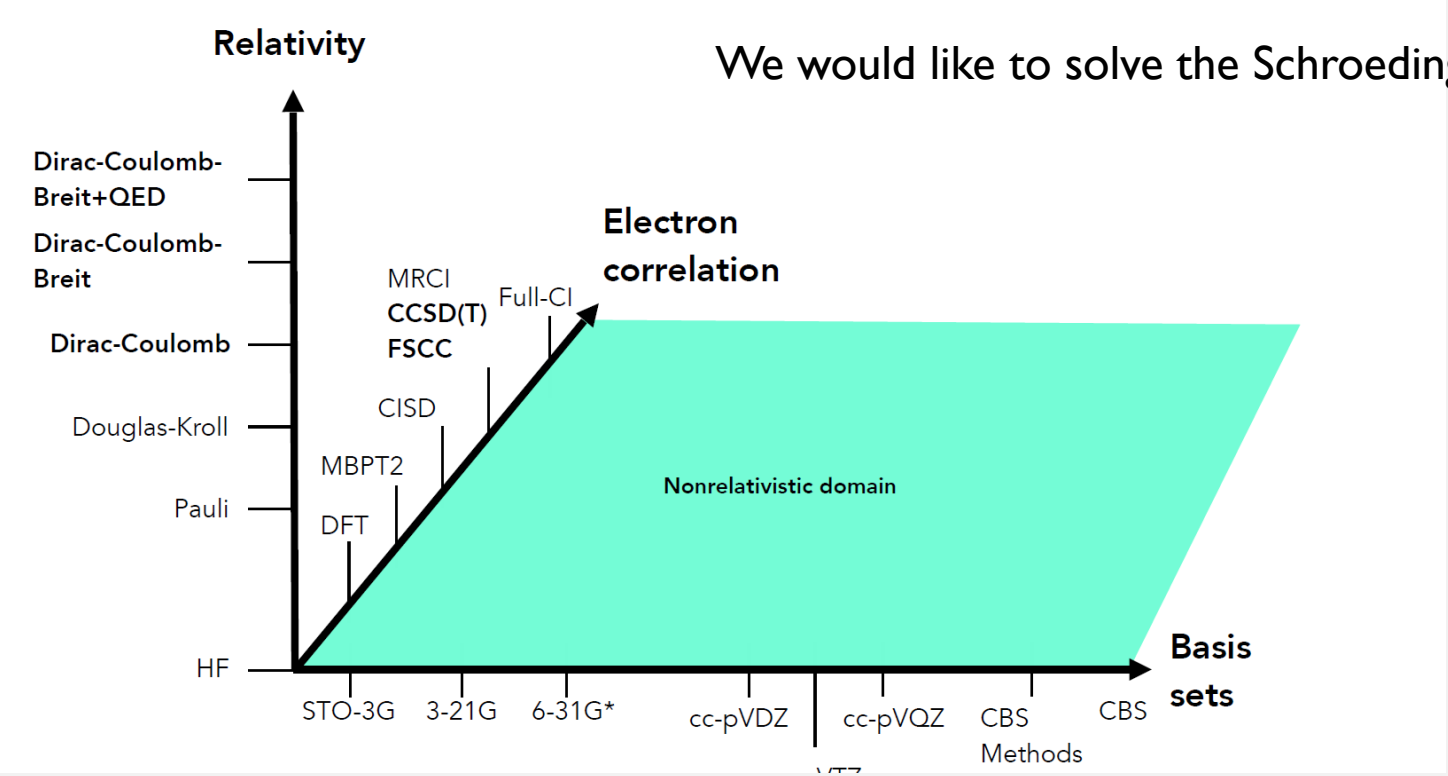
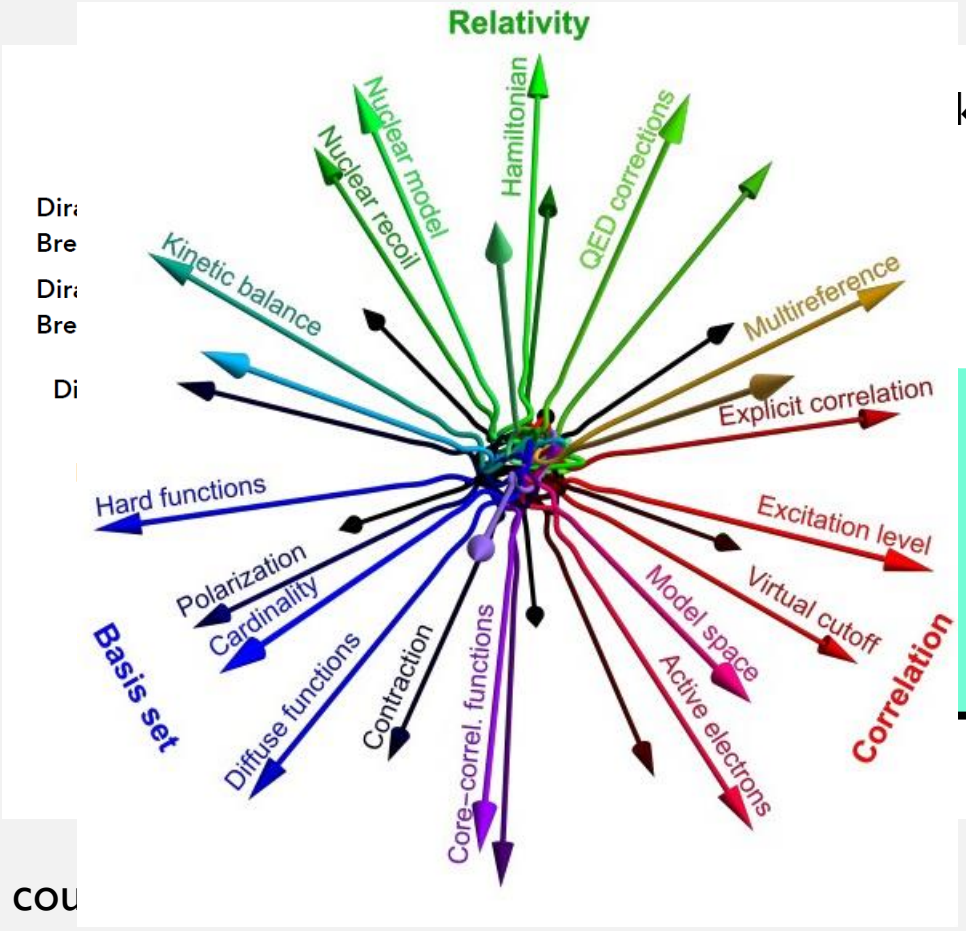


Figure courtesy of P. Schwerdtfeger

COMPUTATIONAL METHODS



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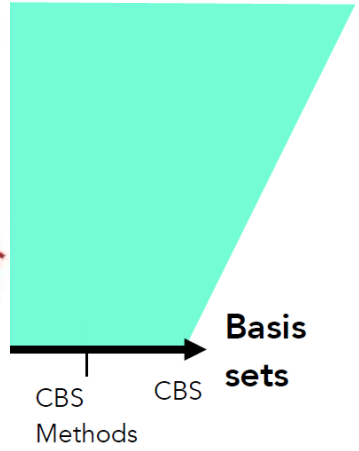
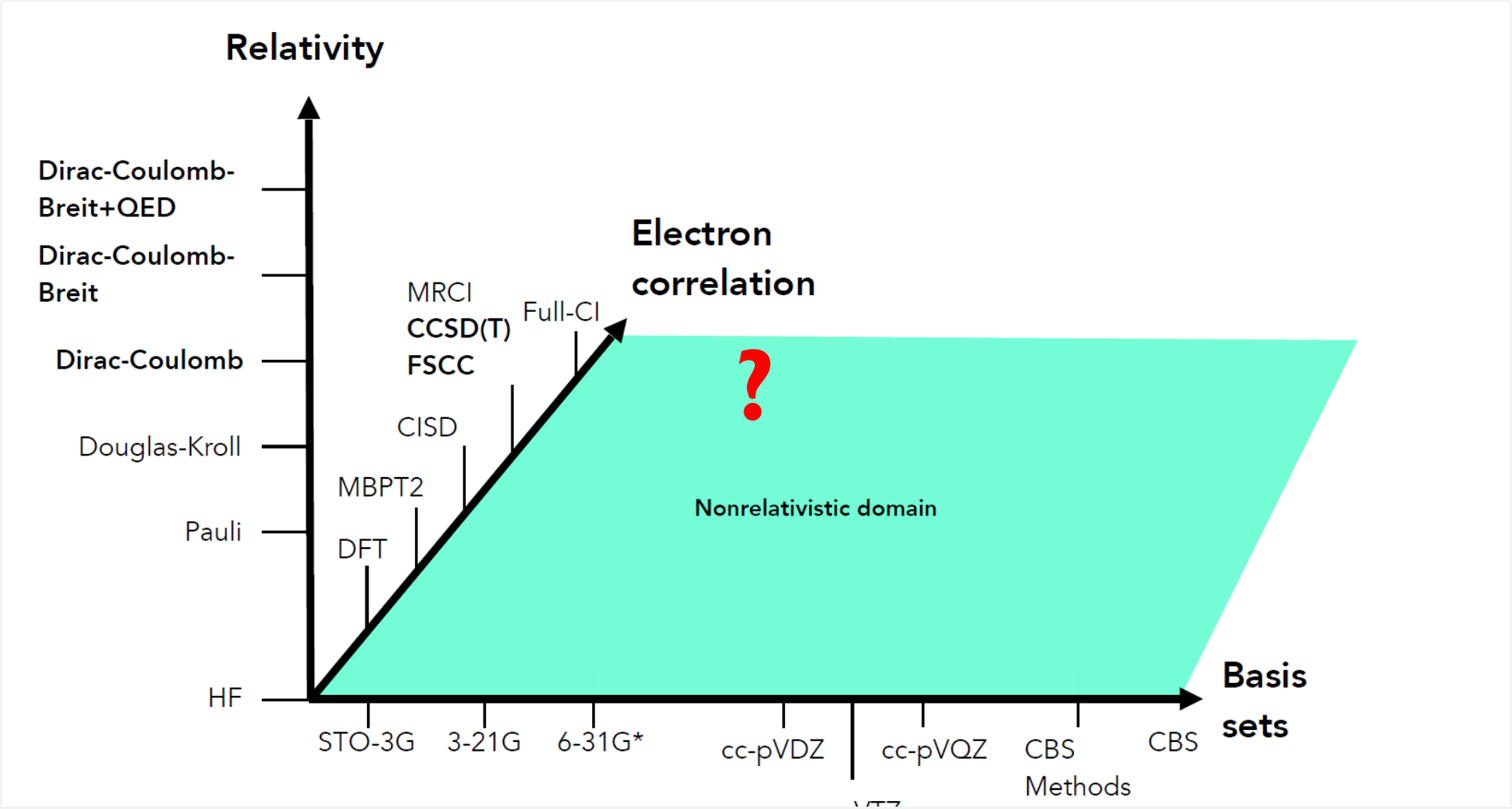
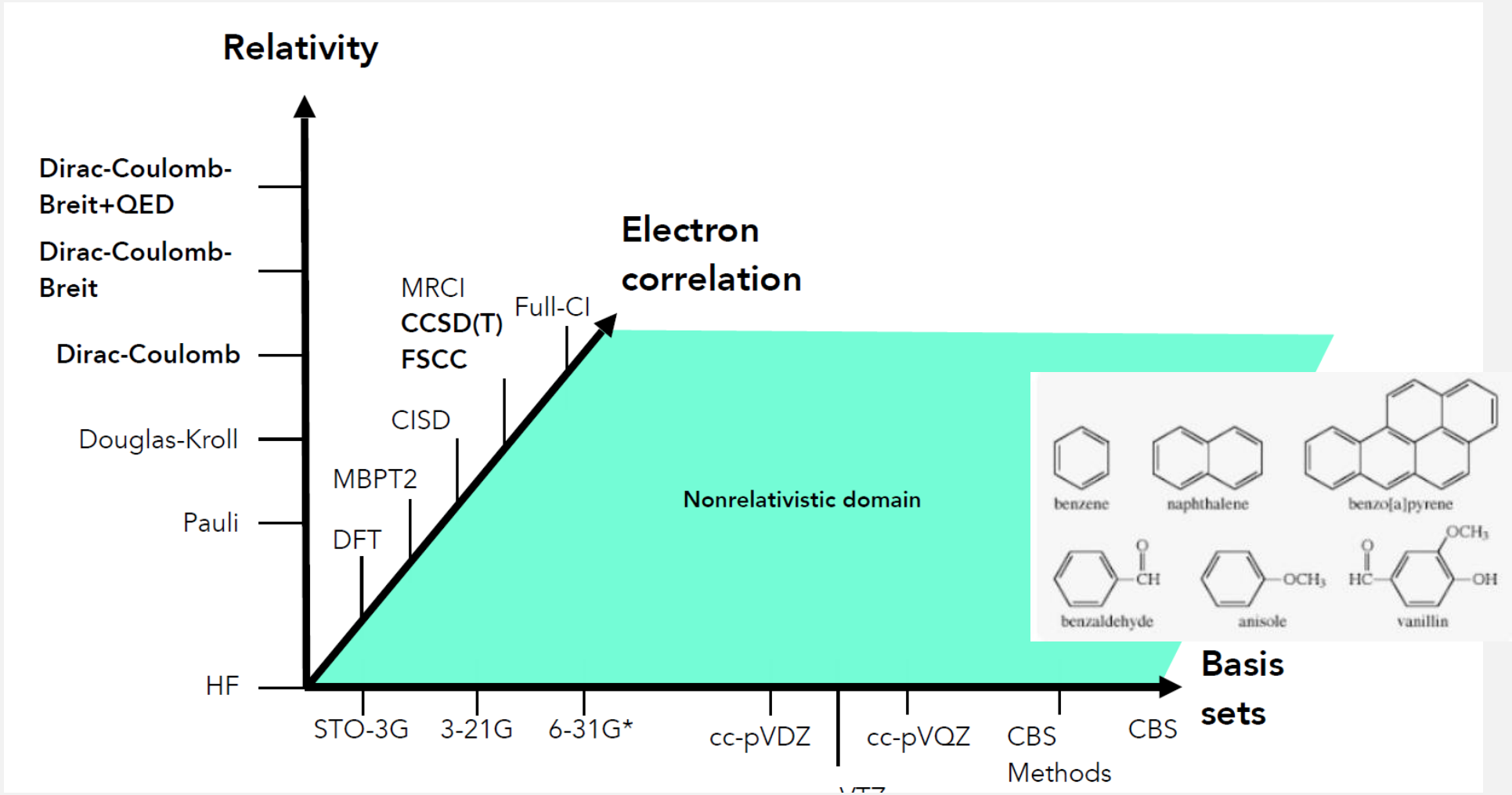


Figure cou


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 want to calculate?

- Coupling parameters describing the effect of *P*(*T*)-violating phenomena on electronic structure
  - Relativistic in nature, hence relativistic methods
- Molecular parameters needed in experiments
  - (usually) heavy systems, hence relativistic methods
-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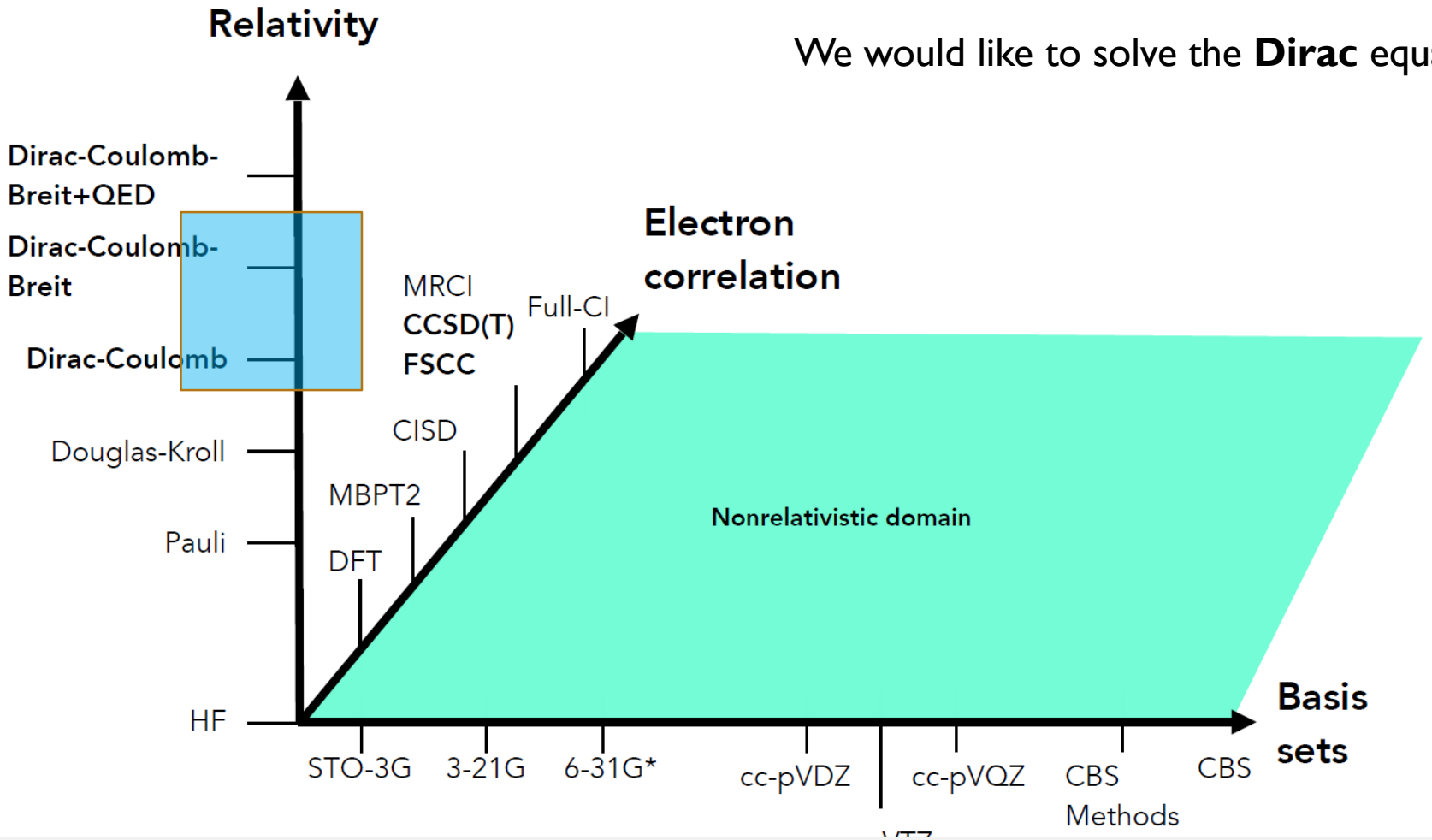
cc-pVQZ
CBS
CBS
Methods
Basis sets
benzene
naphthalene
benzo[a]pyrene
benzaldehyde
anisole
vanillin

We would like to solve the **Dirac** equation.



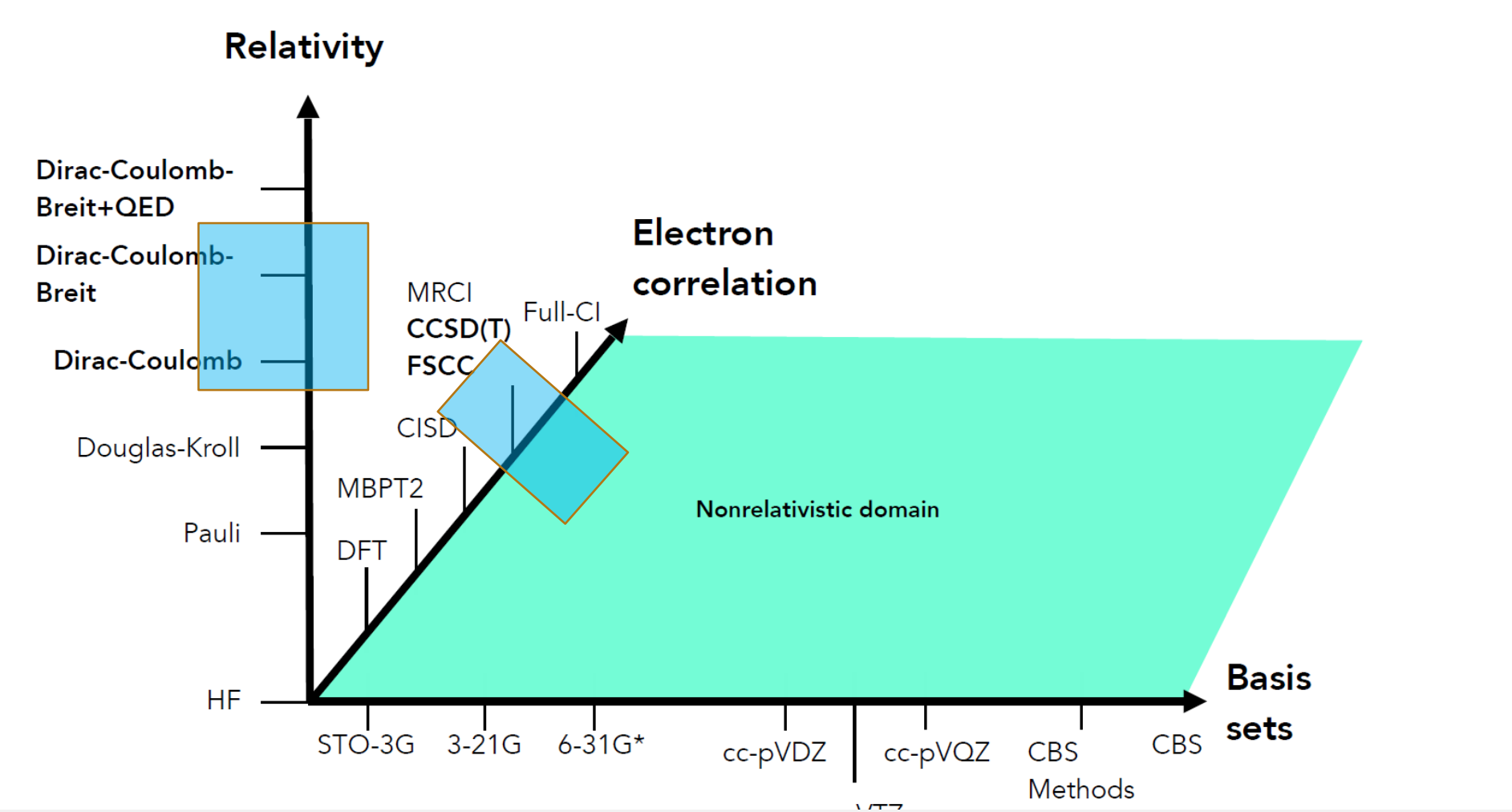
What do we want to calculate?

- Coupling parameters describing the effect of *P*(*T*)-violating phenomena on electronic structure
  - Relativistic in nature, hence relativistic methods
- Molecular parameters needed in experiments
  - (usually) heavy systems, hence relativistic methods
- High accuracy
  - State-of-the-art treatment of correlation
-

Electron correlation

- Explicit interaction between the electrons
- Important for light and heavy elements and for all properties
- Formidable problem, different approaches available
- Our method of choice: **Relativistic coupled cluster (CCSD(T), FSCC)**
- Transparent and robust approach, allows uncertainty estimation

Relativistic coupled cluster

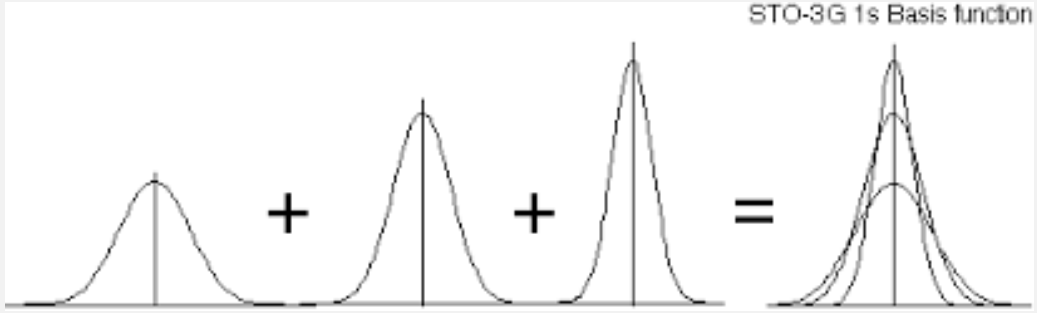


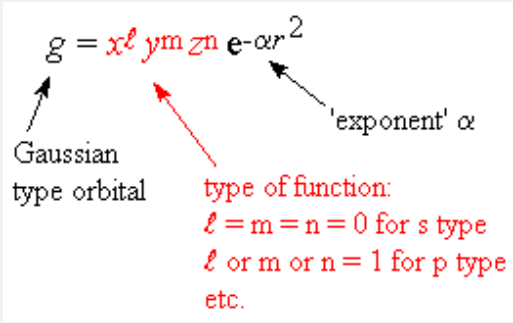
What do we want to calculate?

- 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 systems, hence relativistic methods
- High accuracy
  - State-of-the-art treatment of correlation, large basis sets
-

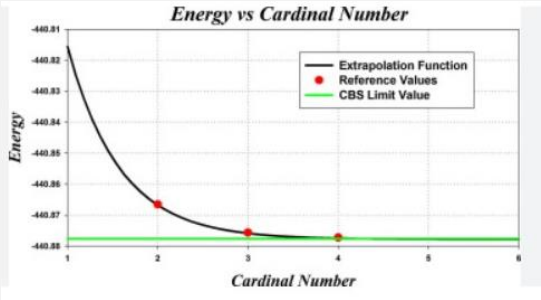
Basis sets (a bit of alchemy)

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



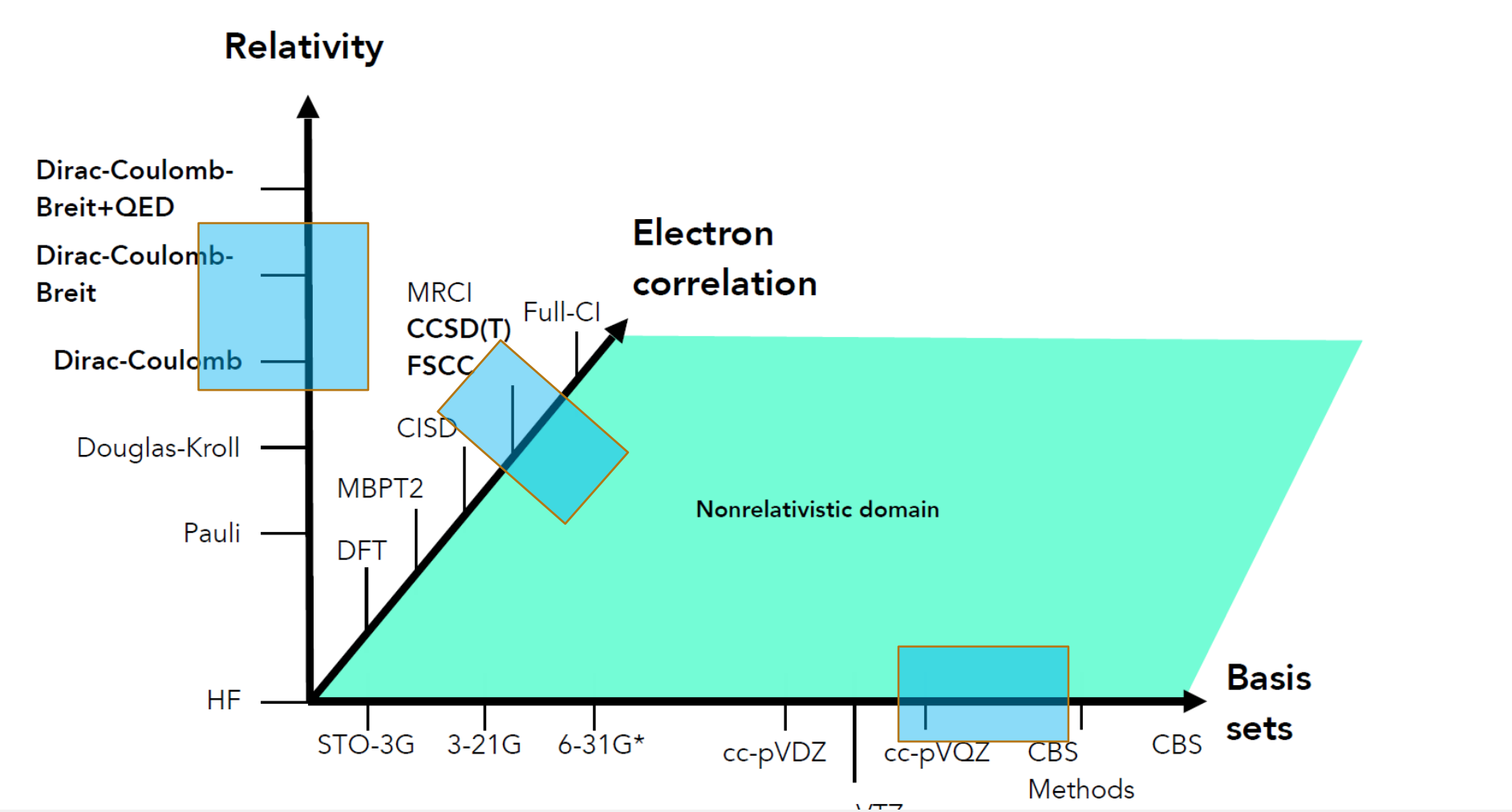


- Dyall's relativistic basis sets
- The larger the basis the better
- Complete Basis Set Limit (CBSL) extrapolation

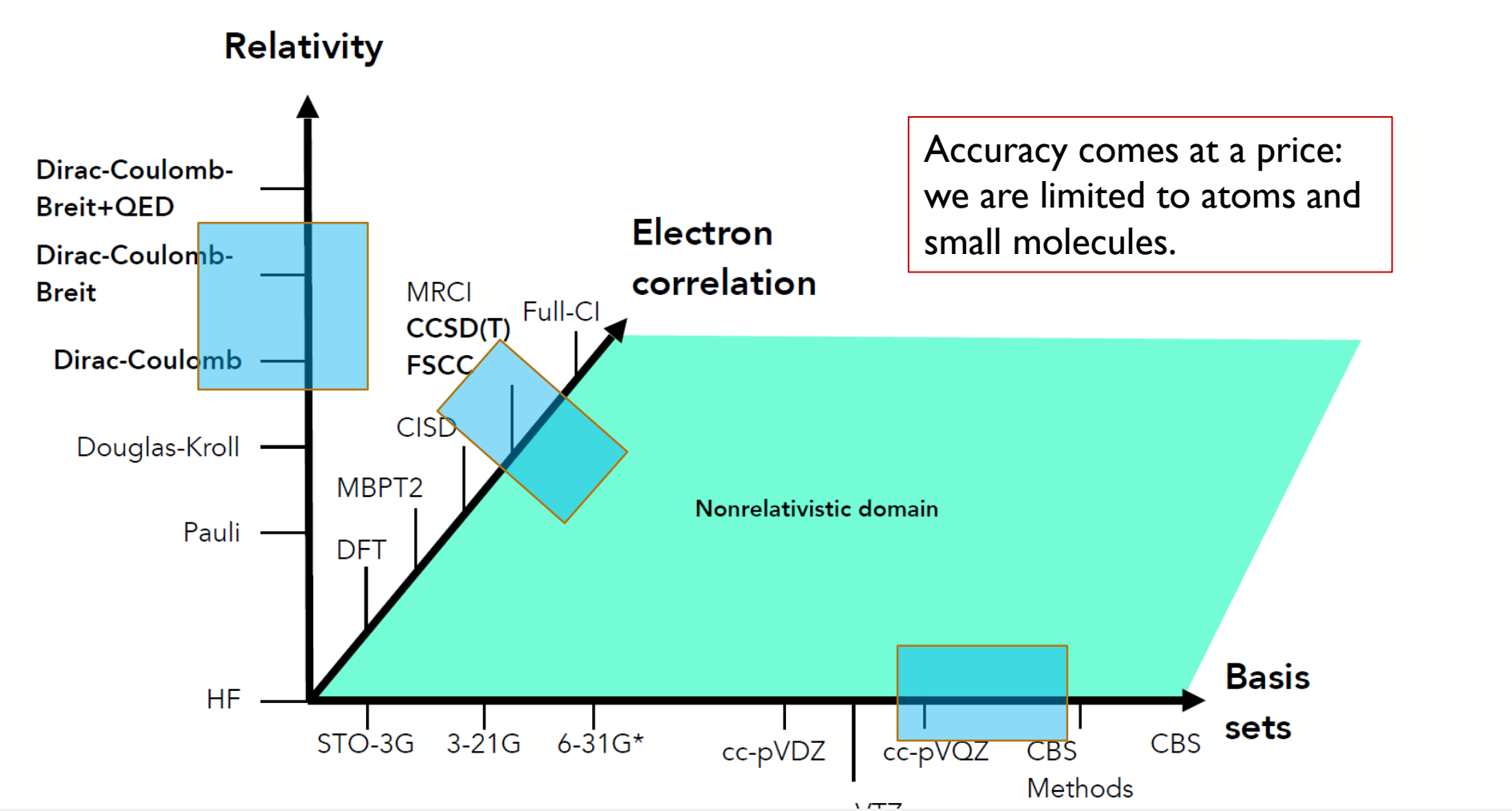


(K.G. Dyall, Theor. Chem Acc. 2002, 2004, 2006, 2007, 2009, 2011,2012, etc.)

Relativistic coupled cluster



Relativistic coupled cluster

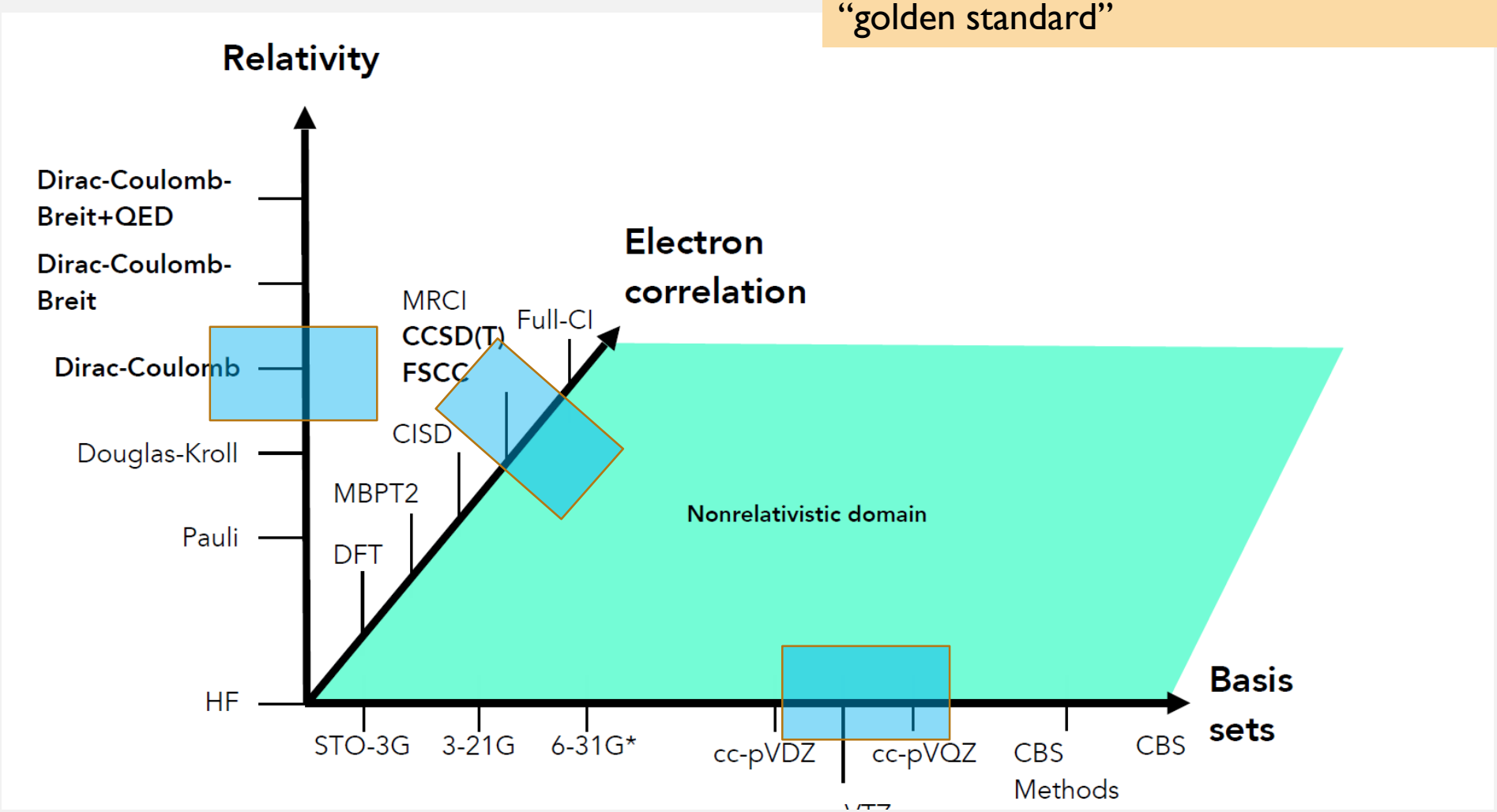


What can we calculate?

- Atomic properties: energies, IPs, EAs, spectra, hyperfine structure parameters, polarisabilities
- Molecular properties: geometries, molecular parameters, electronic structure, Franck-Condon Factors (FCFs), transition strengths
- Properties needed for SM tests:
  - W_d, W_s (eEDM experiments)
  - W_A (NSD-PV, nuclear anapole moments)
  - E_{PV} (parity-violating energy shifts)
  - Sensitivity to variation of α
  - ...
- Ground and excited states; closed and open shells
- Accuracy: ~10s of meV for energies, single % for properties (can be pushed further to meV accuracy)
- Systematic investigation of effect of computational parameters and uncertainty evaluation

How do we reach meV accuracy?

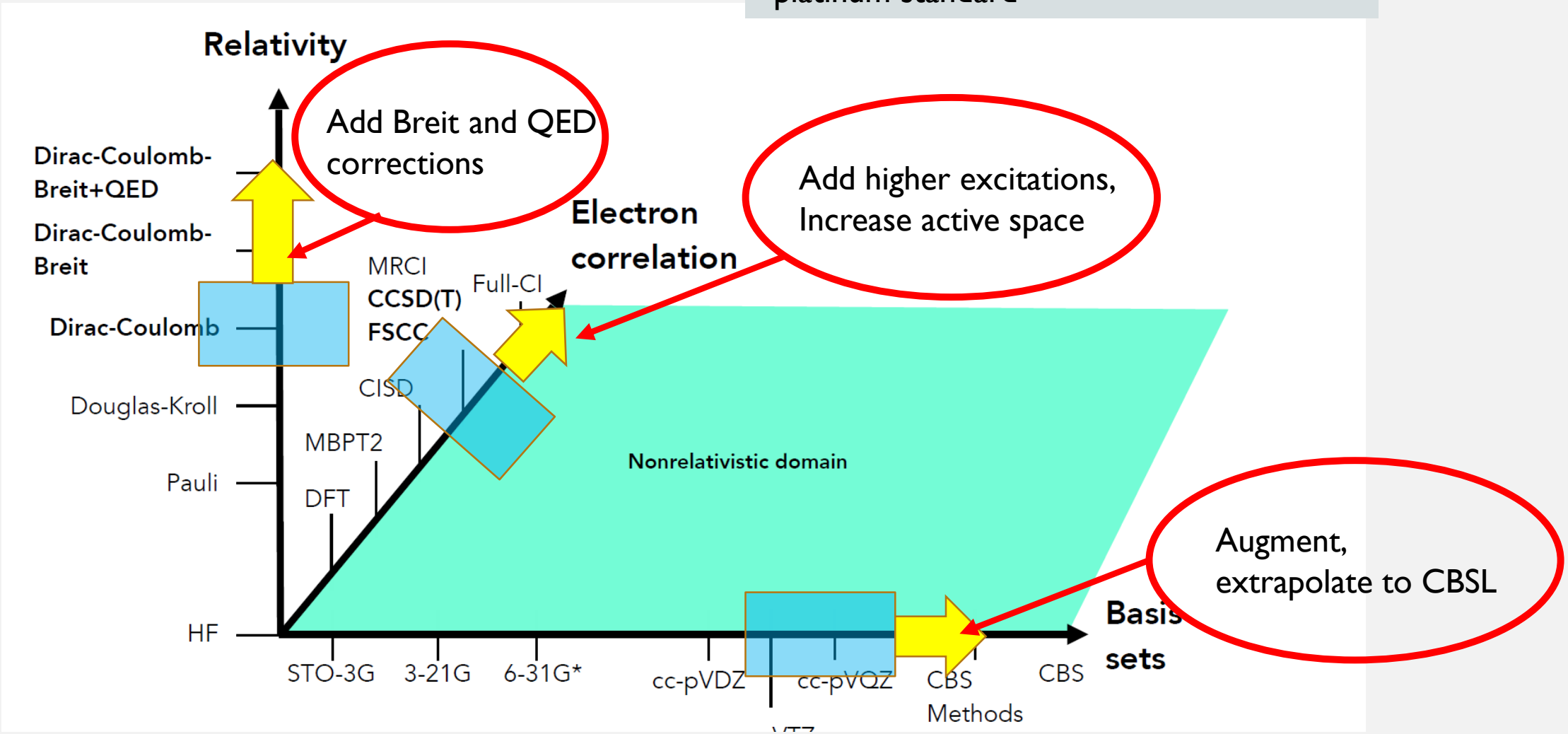
4c-CCSD(T), s-aug-cv4z, active space -20 to 50 a.u.
"golden standard"



4c-CCSD(T), s-aug-cv4z, active space -20 to 50 a.u.
"golden standard"

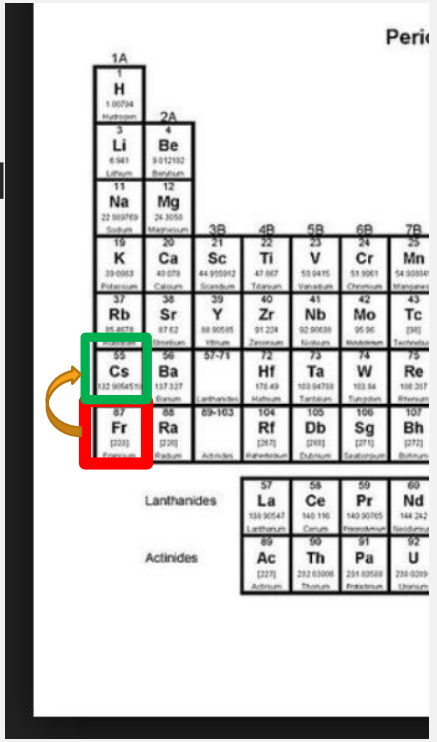
How do we reach meV accuracy?

4c+Breit+QED-CCSDT(Q), CBS limit,
all electrons corelated
"platinum standard"



How do we assign uncertainties (no clear recipe available)?

- Calculate the same property in a lighter homologue (and compare to experiment)
  - E.g., accuracy of the calculated electron affinity in a light element, compared to available experiment, can be used to set error bars on the same property in the heavier homologue
- Calculate a different property in the same atom/molecule (and compare to experiment)
- Perform a computational investigation to assign uncertainties based on method incompleteness



How do we assign uncertainties?

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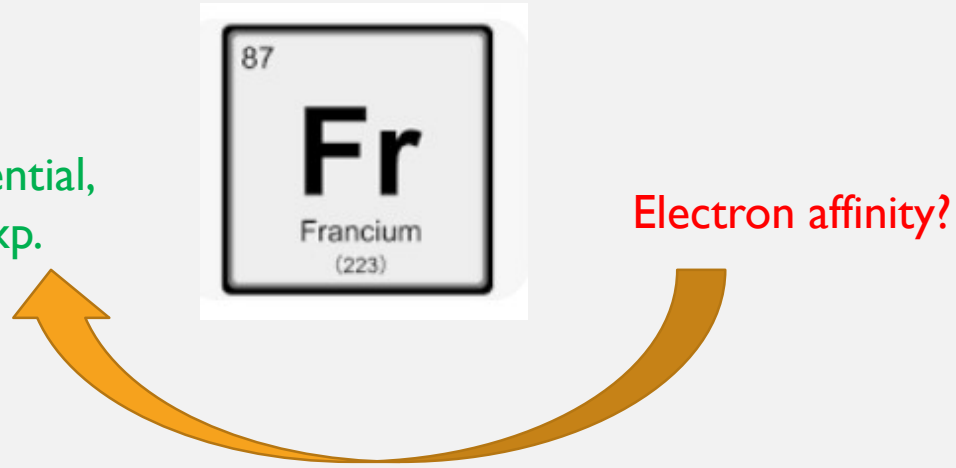
- Calculate a different property in the same atom/molecule (and compare to experiment)
  - E.g., we can use the accuracy of calculated ionization potential in a given element (compared to experiment) to set error bars on the calculated electron affinity in the same atom. Use with caution!
- Perform a computational investigation to assign uncertainties based on method incompleteness



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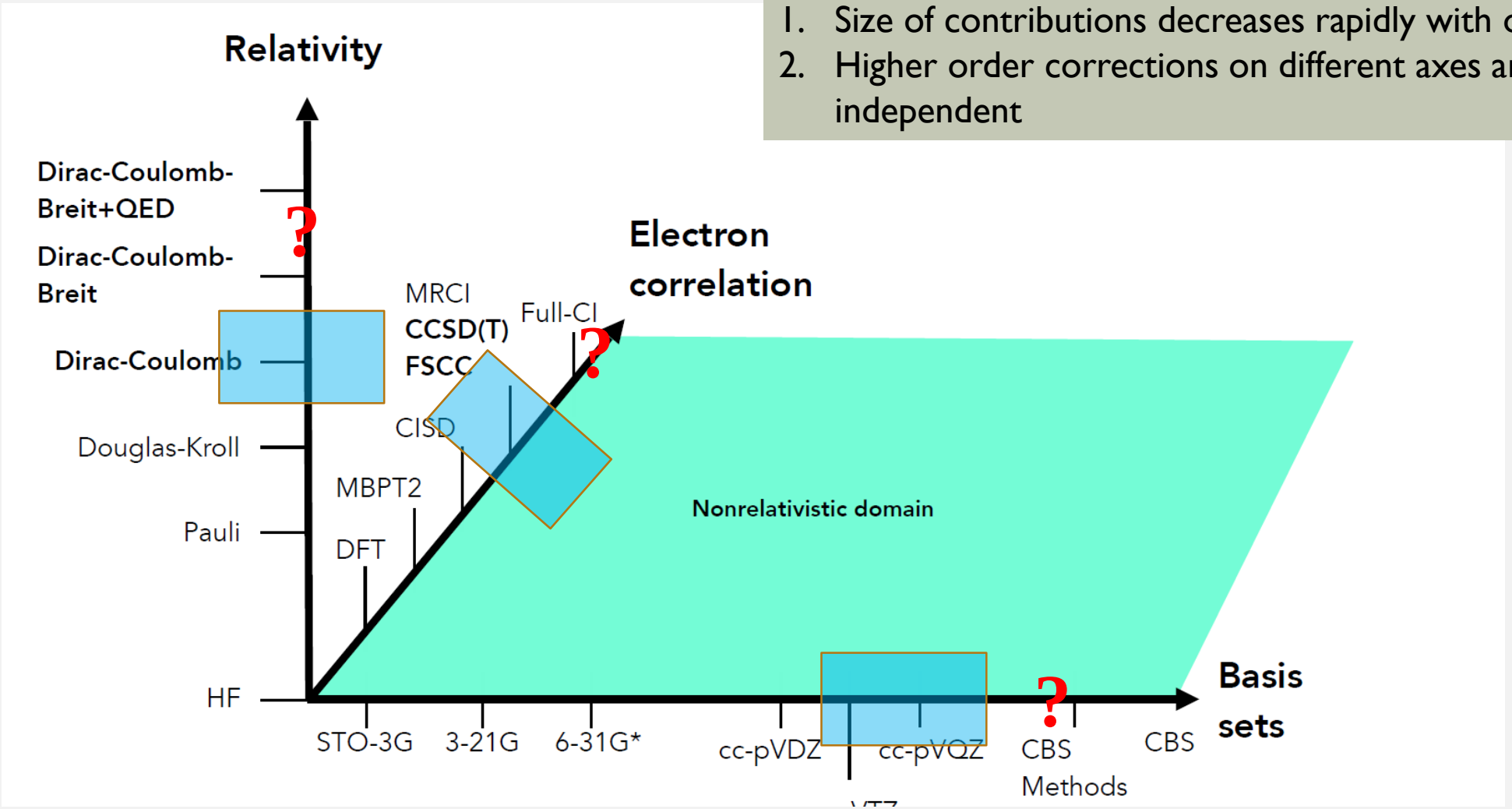
How do we assign uncertainties?

Two assumptions:
1. Size of contributions decreases rapidly with order
2. Higher order corrections on different axes are independent



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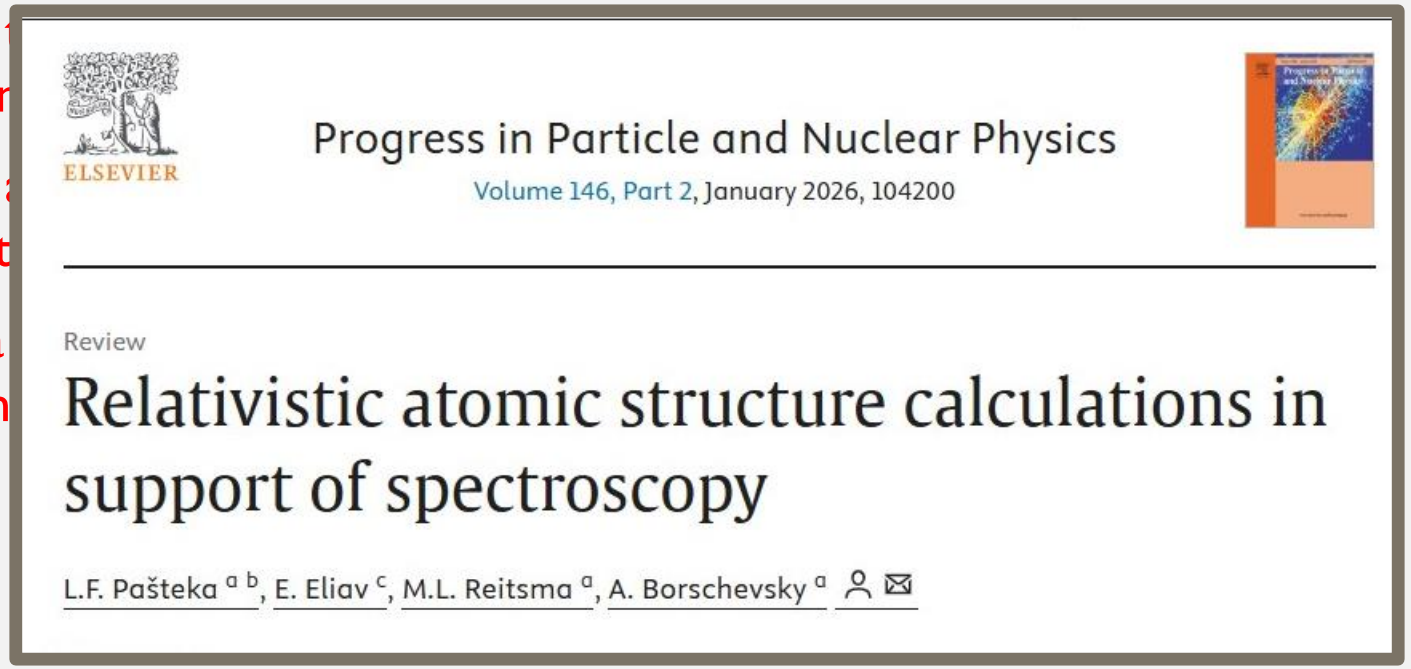
How do we assign uncertainties?

- Calculate
  experimer
- Calculate
  compare t
- Perform a
  method in



ELSEVIER

Progress in Particle and Nuclear Physics

Volume 146, Part 2, January 2026, 104200

Review

Relativistic atomic structure calculations in support of spectroscopy

L.F. Pašteka [a b], E. Eliav [c], M.L. Reitsma [a], A. Borschevsky [a]

TALK OVERVIEW

- Motivation: why do we use atoms and molecules to test the Standard Model?
- Why do we need electronic structure theory?
- How do we perform accurate calculations and assign uncertainties?
- Applications

APPLICATIONS

- Ionization potentials of CaF, SrF, BaF, and RaF: meV accuracy, uncertainty estimation, and predictive power
- P,T-violating coupling constants and molecular parameters
  - Search for the electric dipole moment on the electron: the NL-eEDM collaboration
  - Triatomic molecules: BaOH and YbOH

APPLICATIONS

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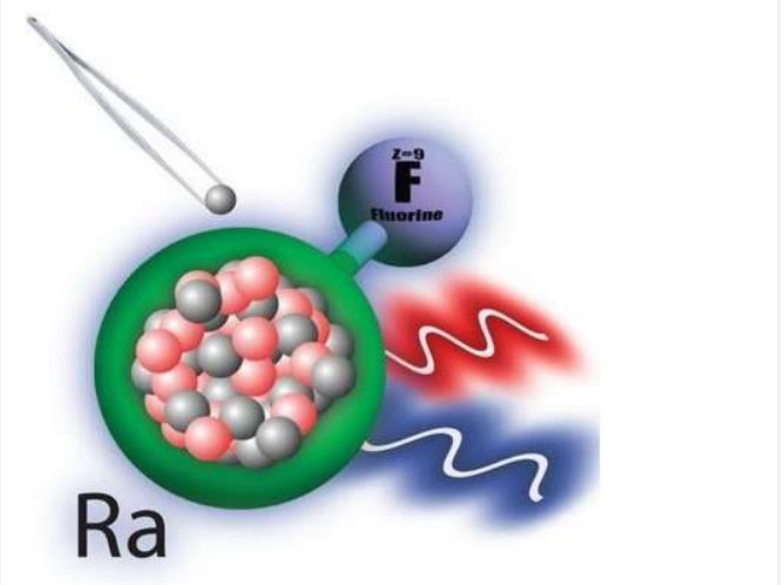
- P,T-violating coupling constants and molecular parameters
  - Search for the electric dipole moment on the electron: the NL-eEDM collaboration
  - Triatomic molecules: BaOH and YbOH

MOLECULAR IONIZATION POTENTIALS

Ionization potential of RaF

- RaF is a promising candidate for new physics searches
- Many (high-impact) experimental studies
- Spectrum, isotope shifts
- New measurements: IP
- Theory before experiment



87. "Precision spectroscopy and laser cooling scheme of a radium-containing molecule".
S.M. Udrescu, S. Wilkins, A. Breier, M. Athanasakis-Kaklamanakis, **R.F. Garcia Ruiz** et al.
Nature Physics (2023).

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Article | Open access | Published: 27 May 2020

Spectroscopy of short-lived radioactive molecules

R. F. Garcia Ruiz, R. Berger, J. Billowes, C. L. Binnersley, M. L. Bissell, A. A. Breier, A. J. Brinson, K. Chrysalidis, T. E. Cocolios, B. S. Cooper, K. T. Flanagan, T. F. Giesen, R. P. de Groote, S. Franchoo, F. P. Gustafsson, T. A. Isaev, Á. Koszorús, G. Neyens, H. A. Perrett, C. M. Ricketts, S. Rothe, L. Schweikhard, A. R. Vernon, K. D. A. Wendt, ... X. F. Yang + Show authors

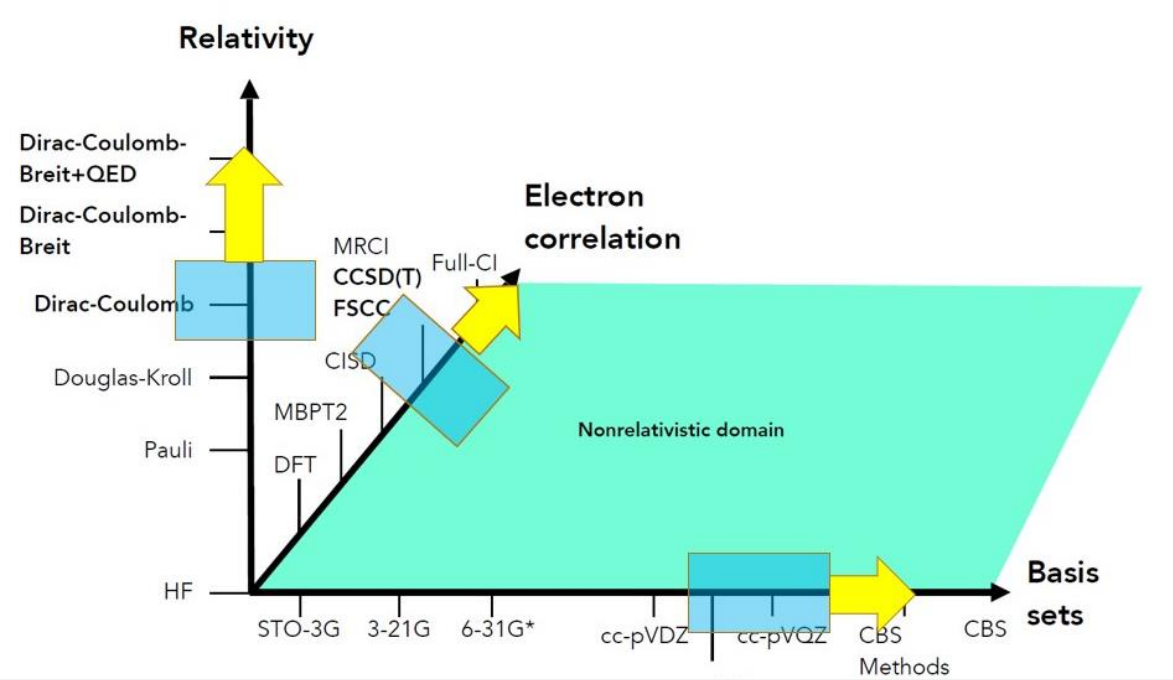
Precision spectroscopy and laser-cooling scheme of a radium-containing molecule

S. M. Udrescu, S. G. Wilkins, A. A. Breier, M. Athanasakis-Kaklamanakis, R. F. Garcia Ruiz, M. Au, I. Belošević, R. Berger, M. L. Bissell, C. L. Binnersley, A. J. Brinson, K. Chrysalidis, T. E. Cocolios, R. P. de Groote, A. Dorne, K. T. Flanagan, S. Franchoo, K. Gaul, S. Geldhof, T. F. Giesen, D. Hanstorp, R. Heinke, Á. Koszorús, S. Kujanpää, ... C. Zülch + Show authors

Nature Physics **20**, 202–207 (2024) | Cite this article

Ionization potential of RaF

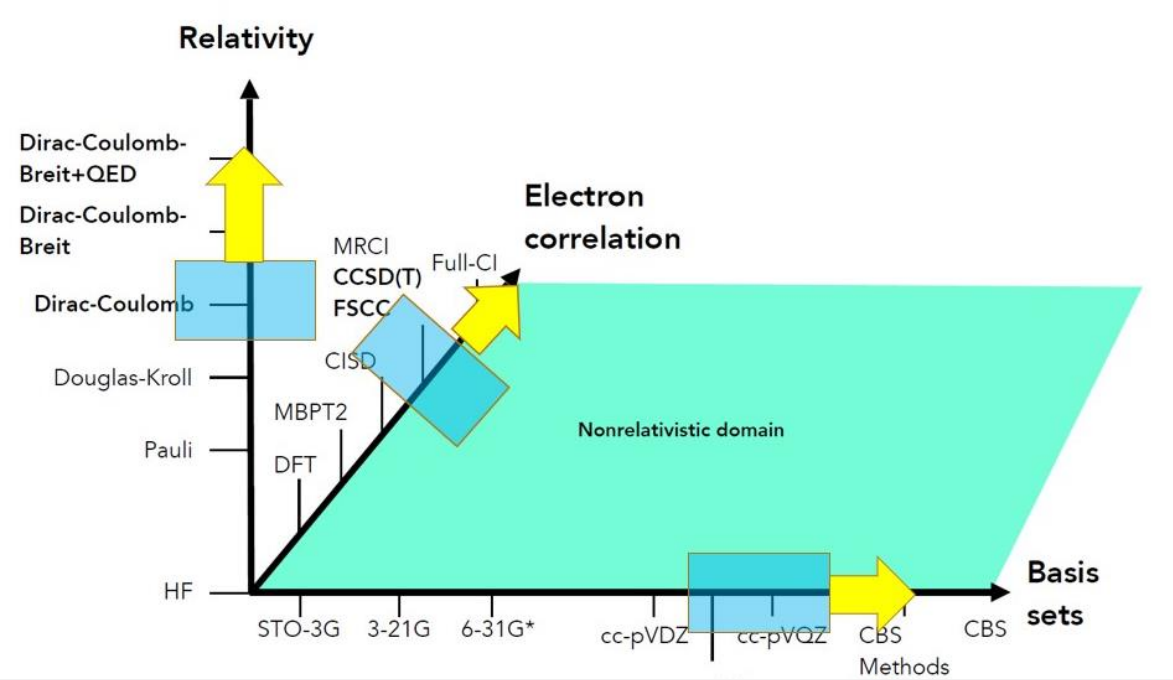
- Theory: relativistic CC with higher order corrections



Method	IP (eV)
CBS-DC-CCSD	4.932[a]
CBS-DC-CCSD(T)	4.983[a]
+augmentation	4.983
+core corr.+active space	4.989
+ΔT	4.990
+Breit	4.988
+QED	4.981
Theoretical	4.981(7)

Ionization potential of RaF

- Theory: relativistic CC with higher order corrections



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Theoretical	4.981(7)

"golden standard"

"platinum standard"

Ionization potential of RaF

- Theory: relativistic CC with higher order corrections
- Uncertainty evaluation: similar contributions from all sources

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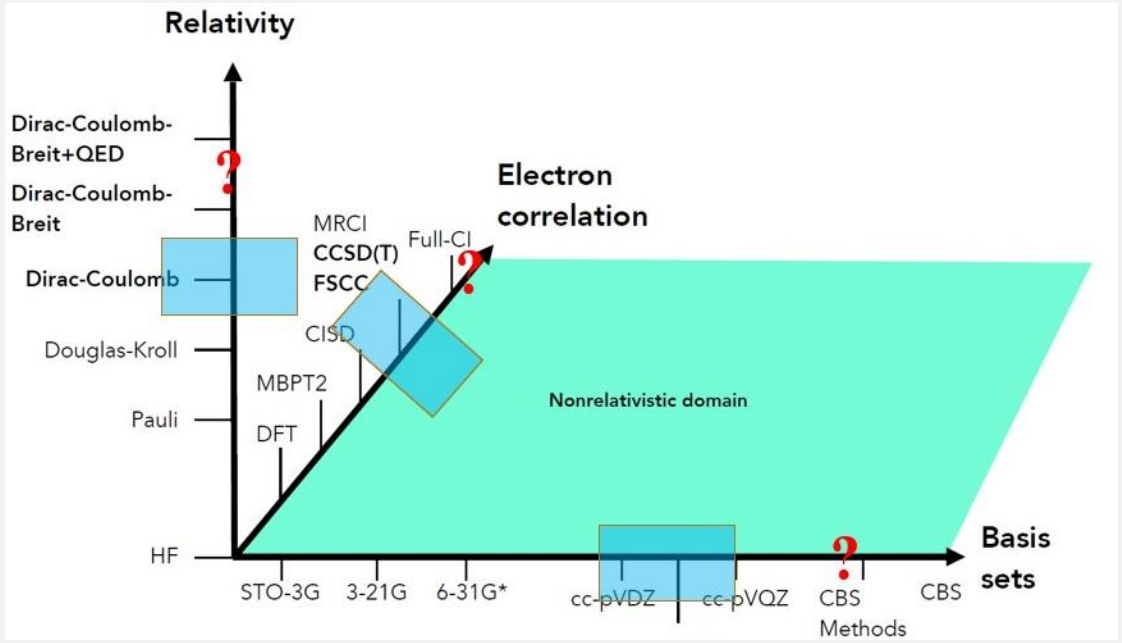

TABLE II. Summary of the main sources of uncertainty in the calculated IP and D_e of RaF.

Category	Error source	IP (meV)
Basis set	Cardinality	2.6
	Augmentation	0.3
Correlation	Core electrons	4.4
	Higher-order excitations	0.9
Relativity	QED	4.2
Uncertainty:		7

How do we assign uncertainties?

- Calculate the same property in a lighter homologue (and compare to experiment)
- Calculate a different property in the same atom/molecule (and compare to experiment)
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Ionization potentials of CaF, SrF, and BaF

- Test the methods on lighter homologues
-

TABLE IV: Calculated IPs of MF (M = Ca,Sr,Ba) [eV] including higher-order contributions.

Method	CaF	SrF	BaF
DC-CCSD	5.8180	5.3940	4.7700
DC-CCSD(T)	5.8236	5.4174	4.8036
+augmentation	–0.0015	0.0003	0.0004
+core corr.+active space	0.0007	–0.0007	–0.0012
+ΔT	0.0005	0.0008	0.0010
+Breit	–0.0010	–0.0011	–0.0009
+QED	–0.0008	–0.0020	–0.0031
Final result	5.8216	5.4148	4.7998

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"golden standard"

"platinum standard"

Ionization potentials of CaF, SrF, and BaF

- Evaluate the weight of different sources of uncertainty
- Here, basis set dominates

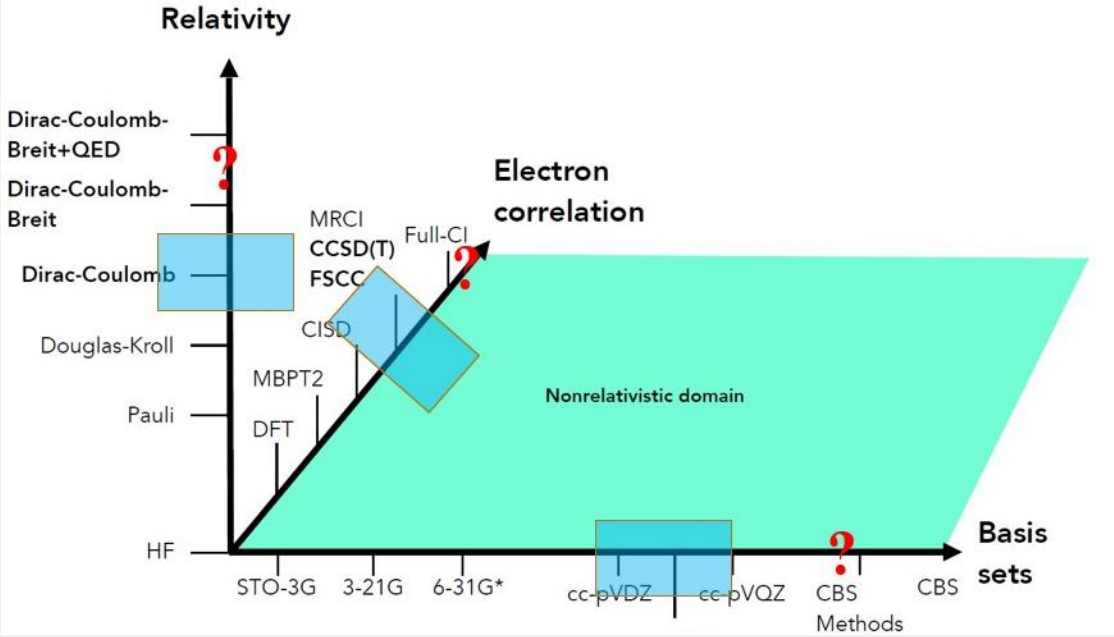

TABLE V: Main sources of uncertainty in the calculated IP of MF (M = Ca, Sr, Ba)[meV].

Category	Error source	CaF	SrF	BaF
Basis set	Cardinality	2.21	1.10	0.50
	augmentation	1.47	0.27	0.37
	inner-core functions	0.01	0.00	2.72
Correlation	virtual space	1.23	0.15	0.44
	higher excitations	0.53	0.84	0.97
Relativity	QED	0.02	0.15	0.52
Total uncertainty, meV		2.97	1.43	3.03

Ionization potentials of CaF, SrF, and BaF

- How accurate are we?
- Excellent agreement for CaF and BaF, where accurate experiment is available
- For SrF, at the time, no accurate experiment was available...
-

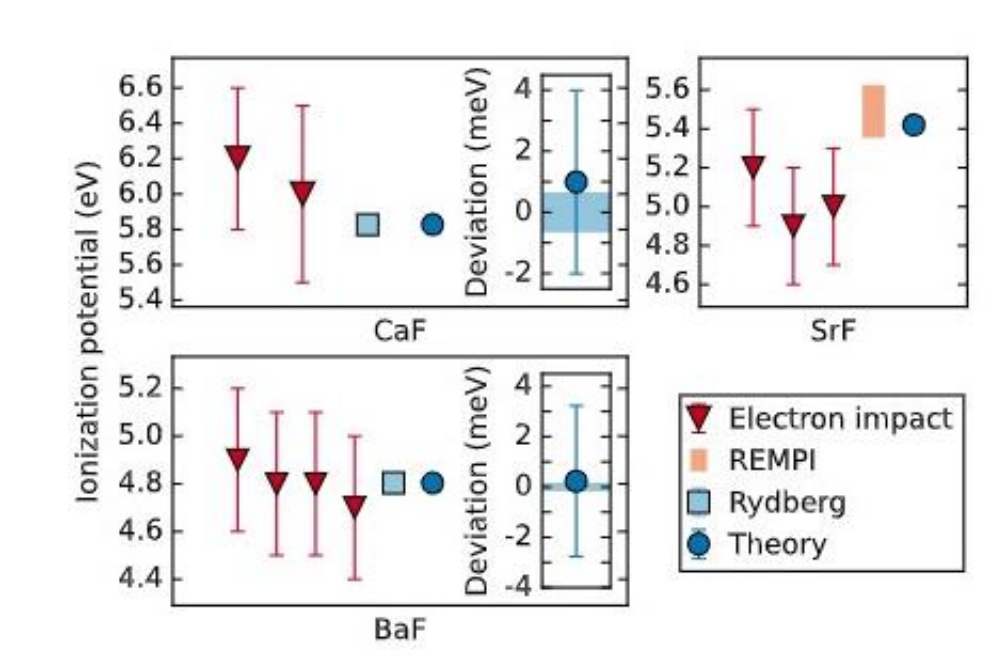

TABLE VI: Recommended theoretical IP of MF (M = Ca, Sr, Ba) [eV] with uncertainties.

IP	CaF	SrF	BaF
Adiabatic	5.821(3)	5.415(1)	4.800(3)
Adiabatic+ZPE	5.828(3)	5.420(1)	4.804(3)
Experiment[a]	5.8270(6)	5.36–5.62	4.80377(1)

[a]-CaF[69], SrF[70] and BaF[39]

Ionization potentials of CaF, SrF, and BaF

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Theoretical determination of the ionization potentials of CaF, SrF, and BaF

A. A. Kyuberis, L. F. Pašteka, E. Eliav, H. A. Perrett, A. Sunaga, S. M. Udrescu, S. G. Wilkins, R. F. Garcia Ruiz, and A. Borschevsky

Phys. Rev. A **109**, 022813 – Published 22 February 2024

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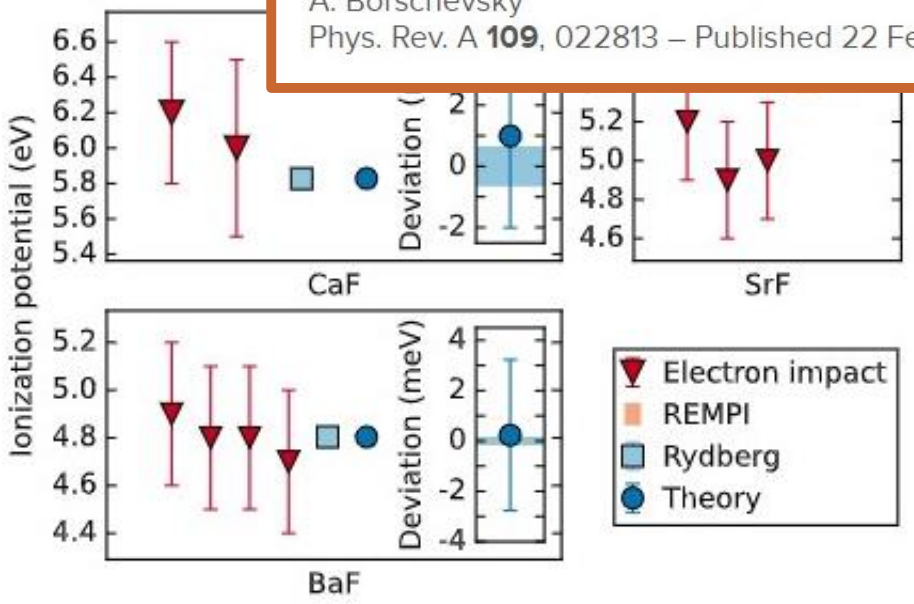

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Back to the ionization potential of RaF

- Measurement: ionization threshold under multi-step laser excitation
- Both two-step and three-step ionization schemes.

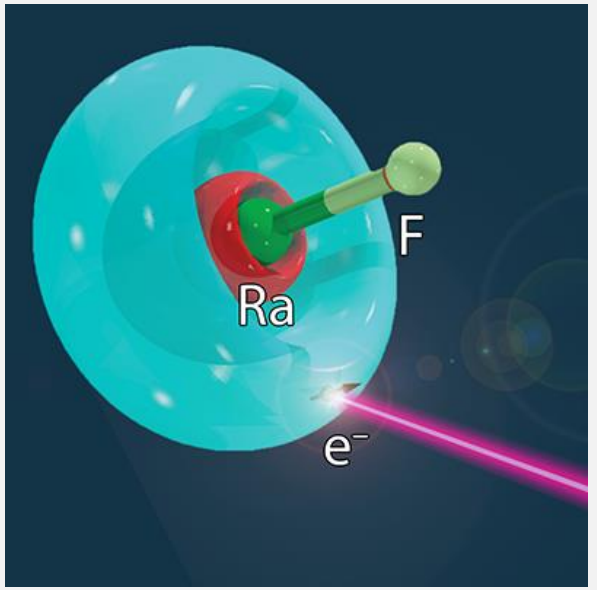
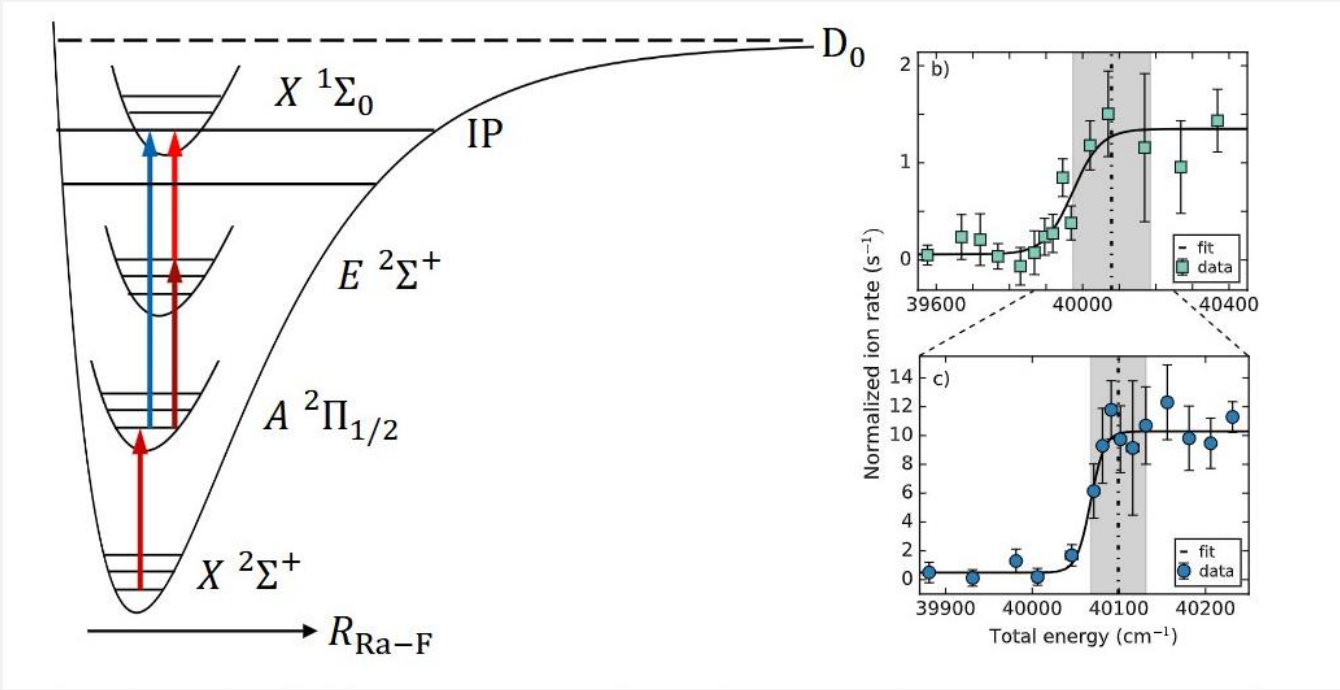


TABLE I. Experimental and calculated IP a

Method	IP (eV)
CBS-DC-CCSD	4.932[a]
CBS-DC-CCSD(T)	4.983[a]
+augmentation	4.983
+core corr.+active space	4.989
+ΔT	4.990
+Breit	4.988
+QED	4.981
Theoretical	4.981(7)
Experimental	



Ionization potential of RaF

- Excellent agreement between theory and experiment
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Ionization potential of RaF

- Excellent agreement between theory and experiment
- Getting the right answer for the right reason

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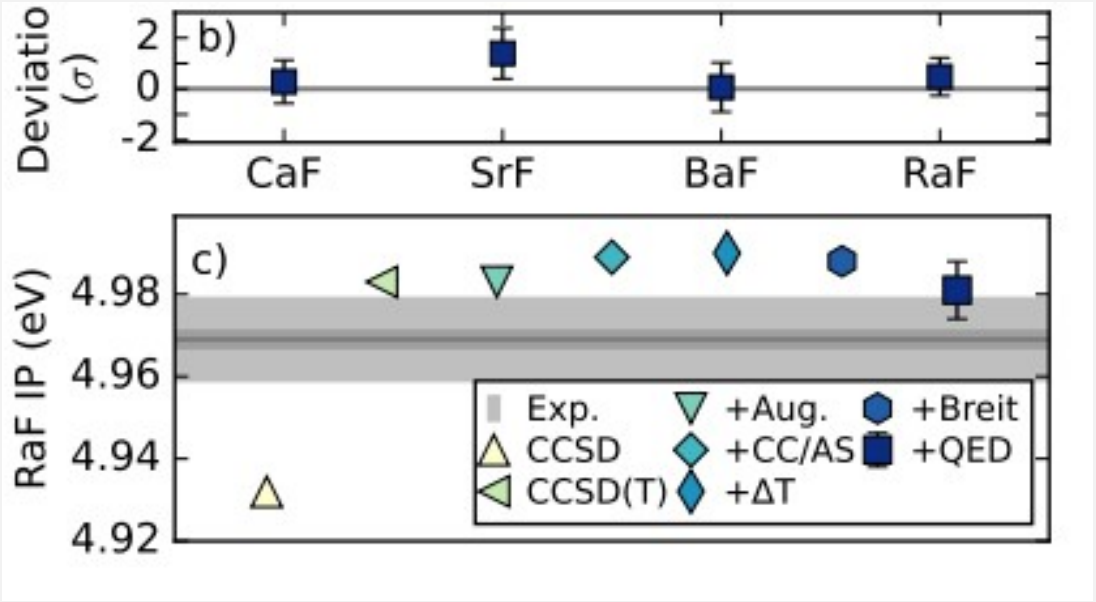

Ionization potential of RaF

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- Relativity in action!

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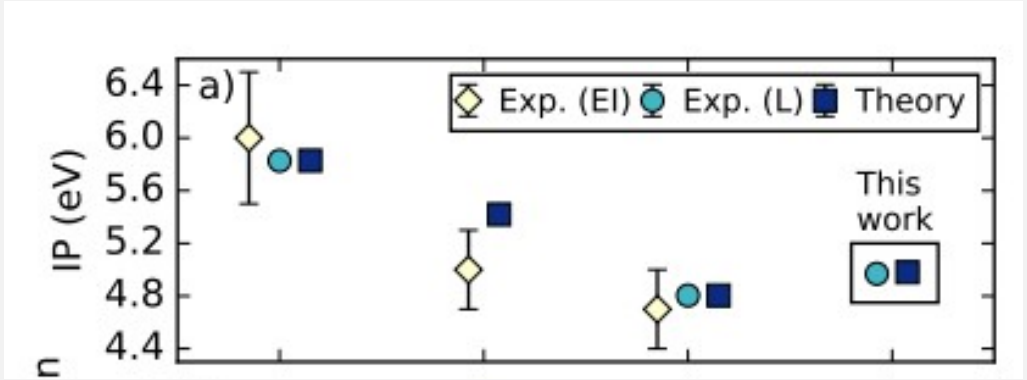

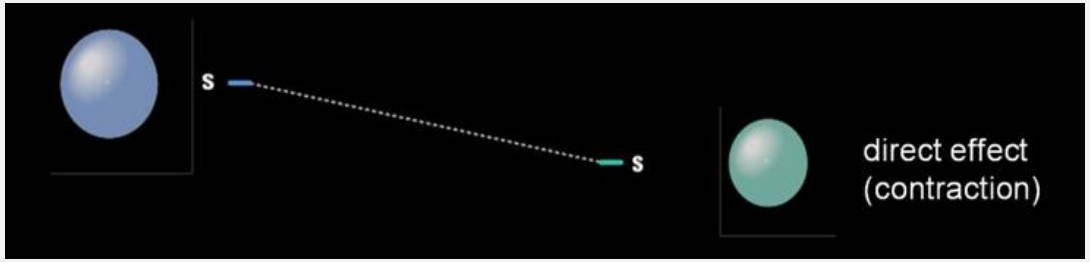

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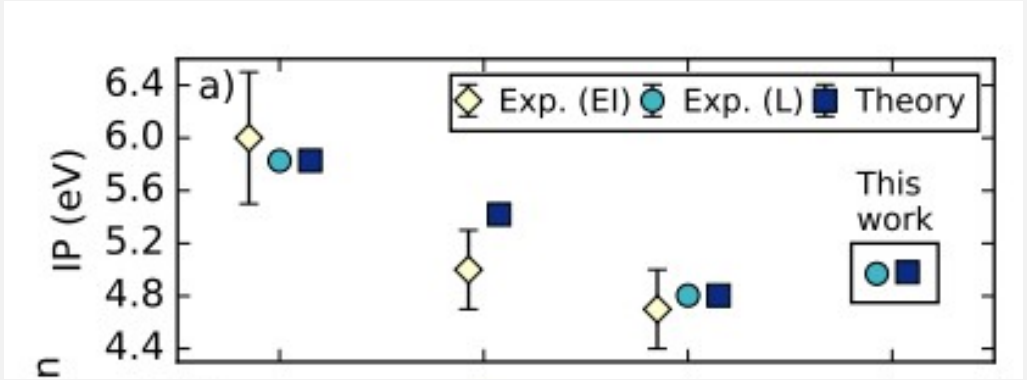

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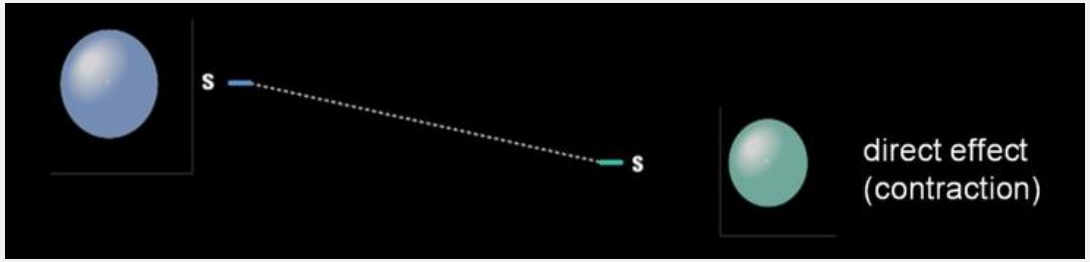
Experimental 4.969(2)[10]

Shane Wilkins, MIT

Aleksandra Kuyberis



Ionization potential of RaF

- Exc
- Get
- Rela

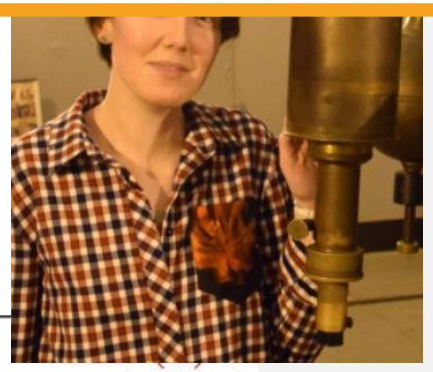
PHYSICAL REVIEW RESEARCH 8, L012012 (2026)

Letter

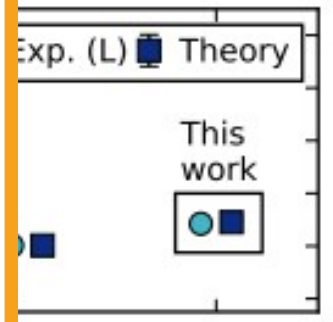
Ionization potential of radium monofluoride

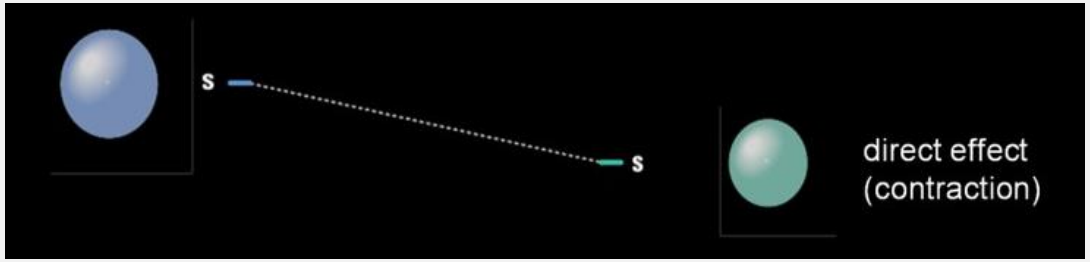
S. G. Wilkins,[1,2,*] H. A. Perrett,[3,†] S. M. Udrescu,[1,‡] A. A. Kyuberis,[4,§] L. F. Pašteka,[4,5] M. Au,[2,6] I. Belošević,[1,7] R. Berger,[8] C. L. Binnersley,[3] M. L. Bissell,[3] A. Borschevsky,[4] A. A. Breier,[9] A. J. Brinson,[1] K. Chrysalidis,[2] T. E. Cocolios,[10] B. S. Cooper,[3] R. P. de Groote,[10] A. Dorne,[10] E. Eliav,[11] R. W. Field,[1] K. T. Flanagan,[12,3] S. Franchoo,[13] R. F. Garcia Ruiz,[1] K. Gaul,[8] S. Geldhof,[10] T. F. Giesen,[9] F. P. Gustafsson,[10] D. Hanstorp,[14] R. Heinke,[2] Á. Koszorús,[2] S. Kujanpää,[15] L. Lalanne,[10] G. Neyens,[10] M. Nichols,[14] J. R. Reilly,[3] C. M. Ricketts,[3] S. Rothe,[2] A. Sunaga,[16,17] B. van den Borne,[10] A. R. Vernon,[3] Q. Wang,[18] J. Wessolek,[3] F. Wienholtz,[2] X. F. Yang,[19] Y. Zhou,[20] and C. Zülch[8]

Shane Wilkins, MIT



Aleksandra Kuyberis





Ionization potentials of CaF, SrF, and BaF

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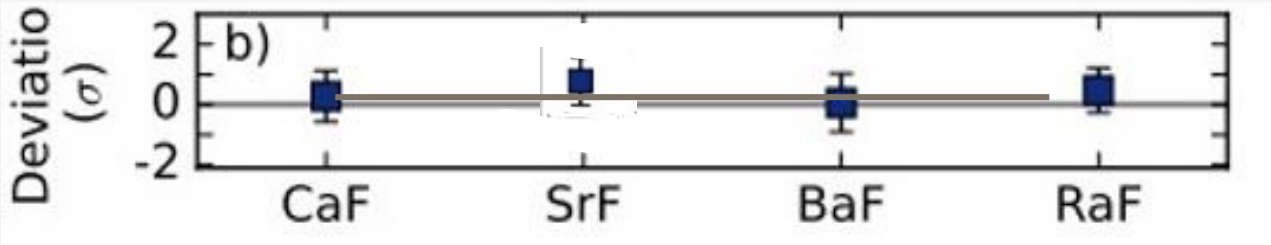
- Excellent agreement for CaF and BaF, where accurate experiment is available
- **For SrF, at the time, no accurate experiment was available...**
- Motivated by our work, measurements were performed in the group of M. Heaven
- The measured IP is just 17 cm^{-1} below the predicted value (5.418(2) eV)



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- *Measurement of the ionization energy of SrF and the vibrational constants of SrF+*

Quynh Giao Lindsey, Jiande Han, Jiayue Lin, Aleksandra A. Kyuberis, and Michael C. Heaven

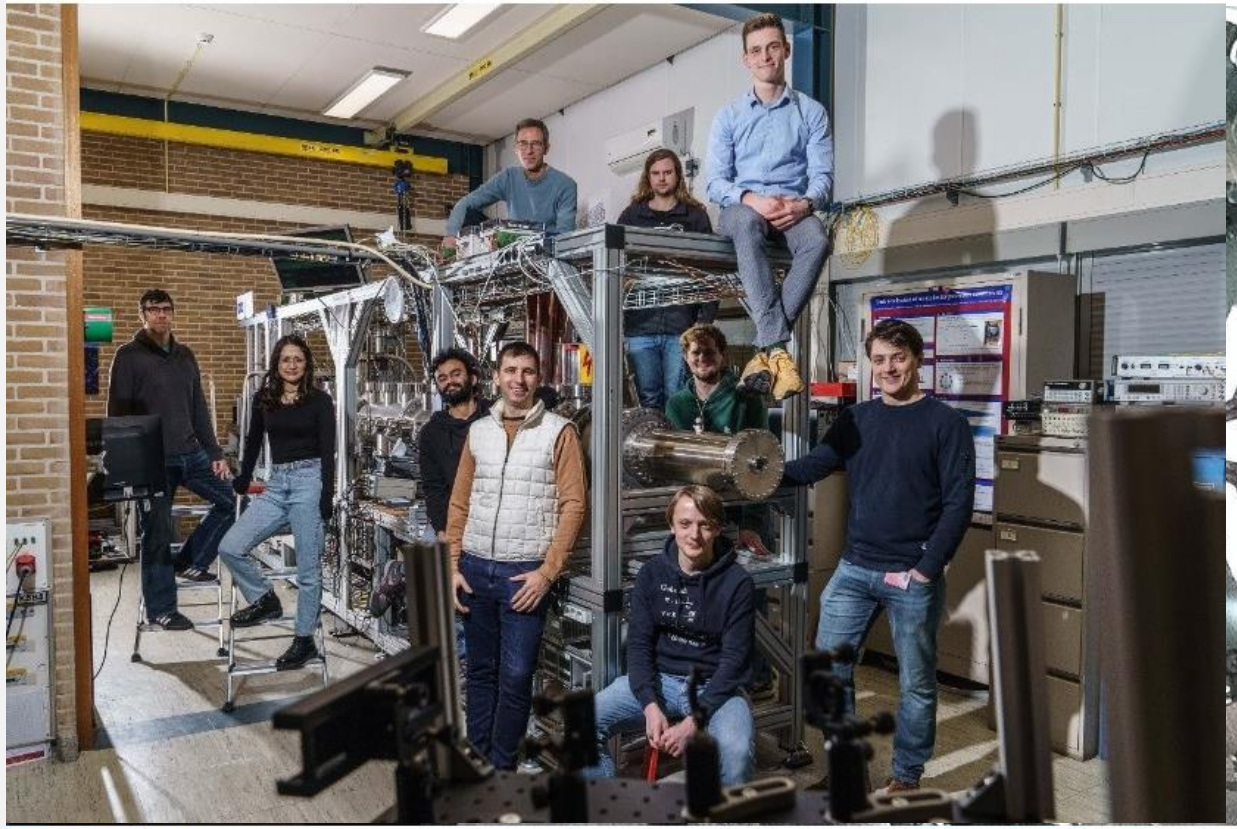
In review

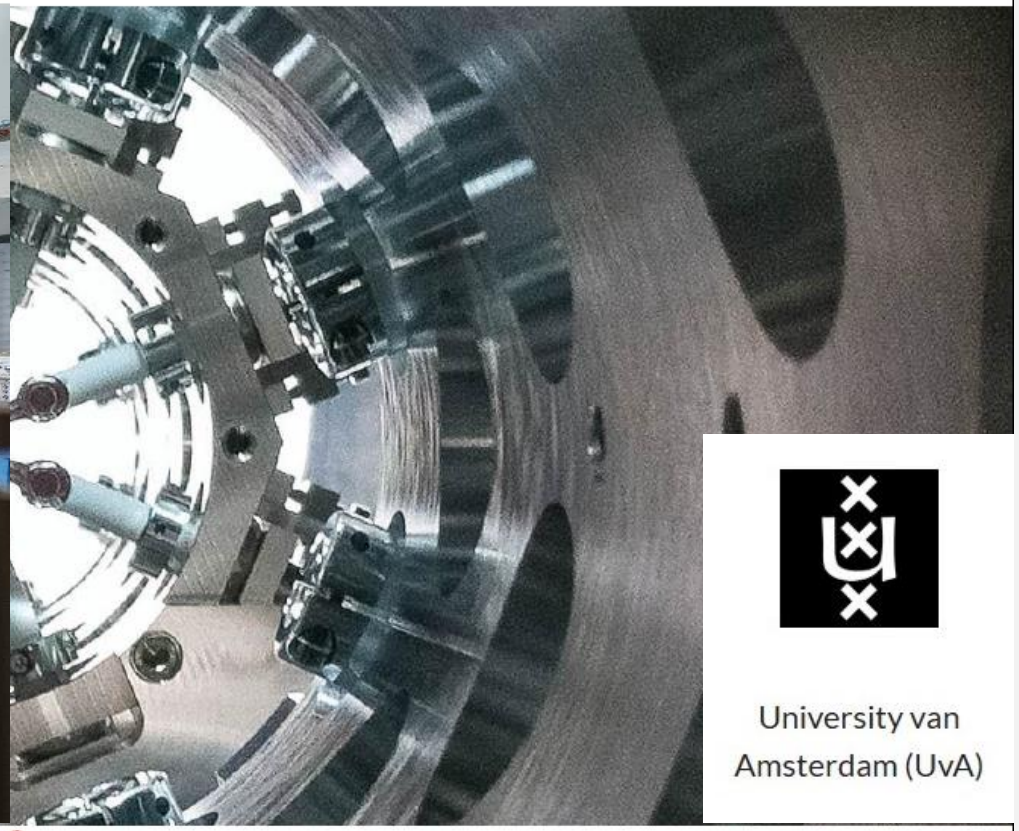
APPLICATIONS

- Ionization potentials of CaF, SrF, BaF, and RaF: meV accuracy, uncertainty estimation, and predictive power
- P,T-violating coupling constants and molecular parameters
  - Search for the electric dipole moment on the electron: the NL-eEDM collaboration
  - Triatomic molecules: BaOH and YbOH

NL-EEDM EXPERIMENT

NL-*e*EDM
Measuring the electron-EDM with BaF molecules





University van Amsterdam (UvA)

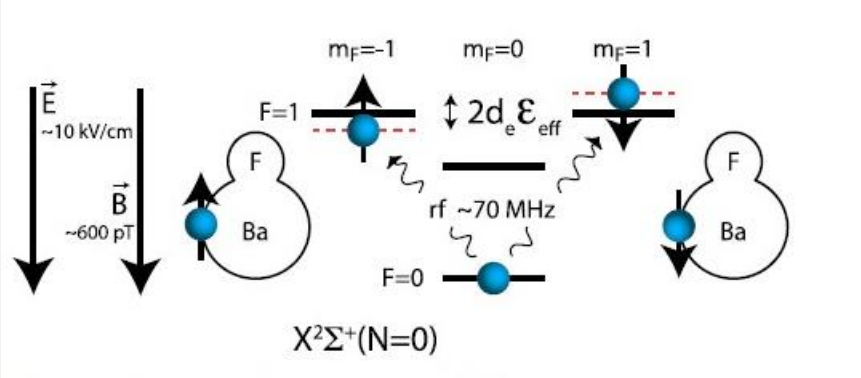
university of groningen
van swinderen institute for particle physics and gravity

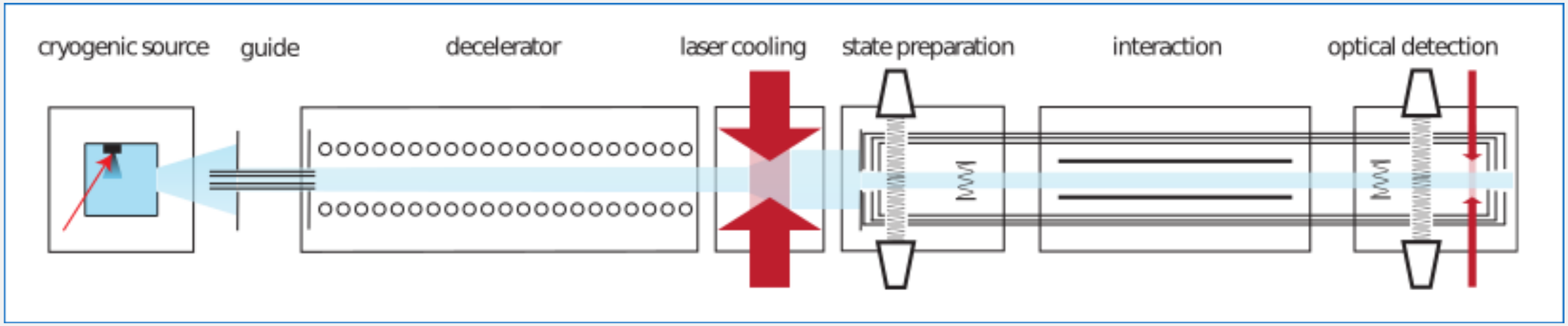
Nikhef
Dutch National Institute for (astro)Particle Physics

VU VRIJE UNIVERSITEIT AMSTERDAM

The experiment:

- The EDM signal is detectable through a difference in the total accumulated phase for the parallel and the antiparallel orientation of the external magnetic and the electric fields.





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Eur. Phys. J. D (2018) 72: 197
https://doi.org/10.1140/epjd/e2018-90192-9

THE EUROPEAN PHYSICAL JOURNAL D

Regular Article

Measuring the electric dipole moment of the electron in BaF

The NL-*e*EDM collaboration: Parul Aggarwal[1,2], Hendrick L. Bethlem[3], Anastasia Borschevsky[1,2], Malika Denis[1,2], Kevin Esajas[1,2], Pi A.B. Haase[1,2], Yongliang Hao[1,2], Steven Hoekstra[1,2,a], Klaus Jungmann[1,2], Thomas B. Meijknecht[1,2], Maarten C. Mooij[2,3], Rob G.E. Timmermans[1,2], Wim Ubachs[3], Lorenz Willmann[1,2], and Artem Zapara[1,2]

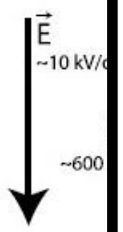
The experiment:

- The EDM sign
  antiparallel or

Statistics and systematics of electron EDM searches with BaF

The NL-*e*EDM collaboration: A. Boeschoten[1,2], V.R. Marshall[1,2], T.B. Meijknecht[1,2], A.P. Touwen[1,2], P. Aggarwal[1,2], N. Balasubramanian[1,2], R. Bause[1,2], H. L. Bethlem[1,3], A. Borschevsky[1,2], T.H. Fikkers[1,2], P.A.B. Haase[1,2], Y. Hao[1], S. Hoekstra[1,2], J.W.F. van Hofslot[1,2], S.A. Jones[1,2], K. Jungmann[1], J.E.J. Levenga[1,2], M.C. Mooij[2,3], H. Mulder[1,2], B.A. Nijman[1,2], E.H. Prinsen[1,2], B.J. Schellenberg[1,2], I.E. Thompson[1,2], R.G.E. Timmermans[1,2], L. van Sloten[1,2], W. Ubachs[3], J. de Vries[2,4], L. Willmann[1,2], Y. Yin[1,2]

arXiv:2601.21781



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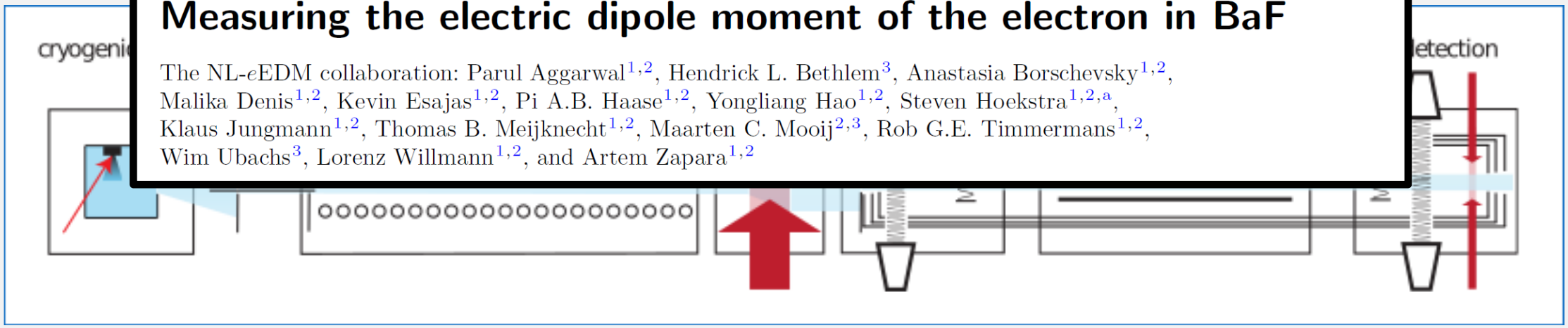


Interpreting the experiment: 2 sources of *P,T*-effects

$$\hat{H}^{\mathrm{P,T}} = (W_d d_e + W_s k_s)\hat{\mathbf{S}} \cdot \hat{\mathbf{n}}$$

What we want

$$\Delta E = (W_d d_e + W_s \kappa_s) < \hat{S} \cdot \hat{n} > (E_{\mathrm{ext}})$$

measured

Have to come from calculations

d_e- electron EDM, κ_s - *S-PS* electron-nucleon interaction

Electric dipole moments: A global analysis

Timothy Chupp and Michael Ramsey-Musolf
Phys. Rev. C **91**, 035502 – Published 6 March 2015

Investigations of optimal combinations of molecules:

- K. Gaul, S. Marquardt, T. Isaev, and R. Berger, Phys. Rev. A **99**, 032509 (2019)
- A . Sunaga, M. Abe, V. S. Prasannaa, T. vAoki, and M. Hada, J. Phys. B **53**, 015102 (2019)

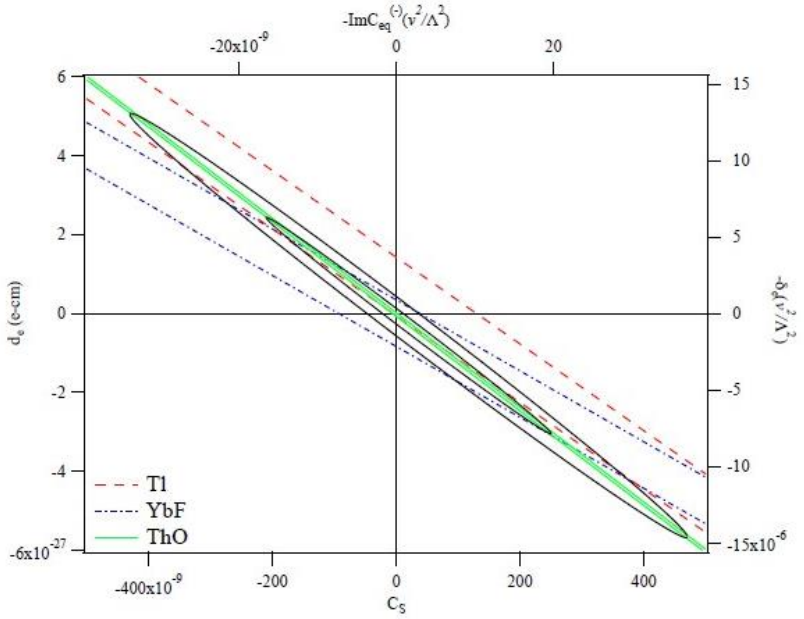


FIG. 1: Electron edm d_e as a function of C_S from the experimental results in Tl, YbF and ThO. Also shown are 68% and 95% error ellipses representing the best-fit for the paramagnetic systems and including $d_A(^{199}\mathrm{Hg})$ as discussed in the text. Also shown are the constraints on the dimensionless Wilson coefficients δ_e and $\mathrm{Im}\,C_{eq}^{(-)}$ times the squared scale ratio $(v/\Lambda)^2$.

Interpreting the experiment: 2 sources of *P,T*-effects

$$\hat{H}^{\mathrm{P,T}} = (W_d d_e + W_s k_s)\hat{\mathbf{S}} \cdot \hat{\mathbf{n}}$$

$$H^{\mathrm{EDM}} = 2cd_e \sum_{i=1}^{n} \imath\gamma^0(i)\gamma^5(i)\mathbf{p}^2(i)$$

$$W_d = \frac{1}{d_e} \langle \psi_\Omega | H^{\mathrm{EDM}} | \psi_\Omega \rangle$$

$$H_S = i\frac{G_F}{\sqrt{2}} Z\kappa_S \sum_{i=1}^{n} \gamma^0\gamma^5\rho_A(r_i)$$

$$W_S = \frac{1}{\kappa_S} \frac{1}{\Omega} \langle \psi_\Omega | H_S | \psi_\Omega \rangle$$

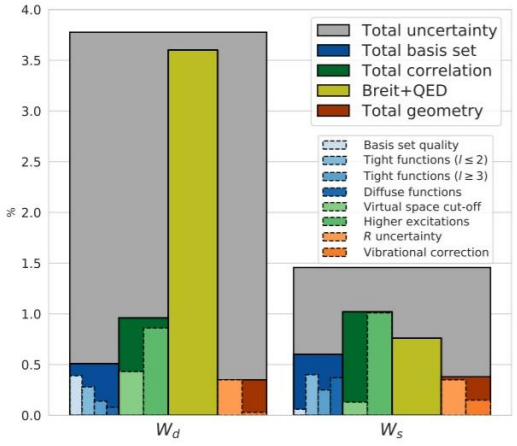
- Use relativistic CC (Finite Field) to calculate W_d and W_s.
- Systematically improve the calculation up to convergence
- Perform an extensive computational study to estimate uncertainties

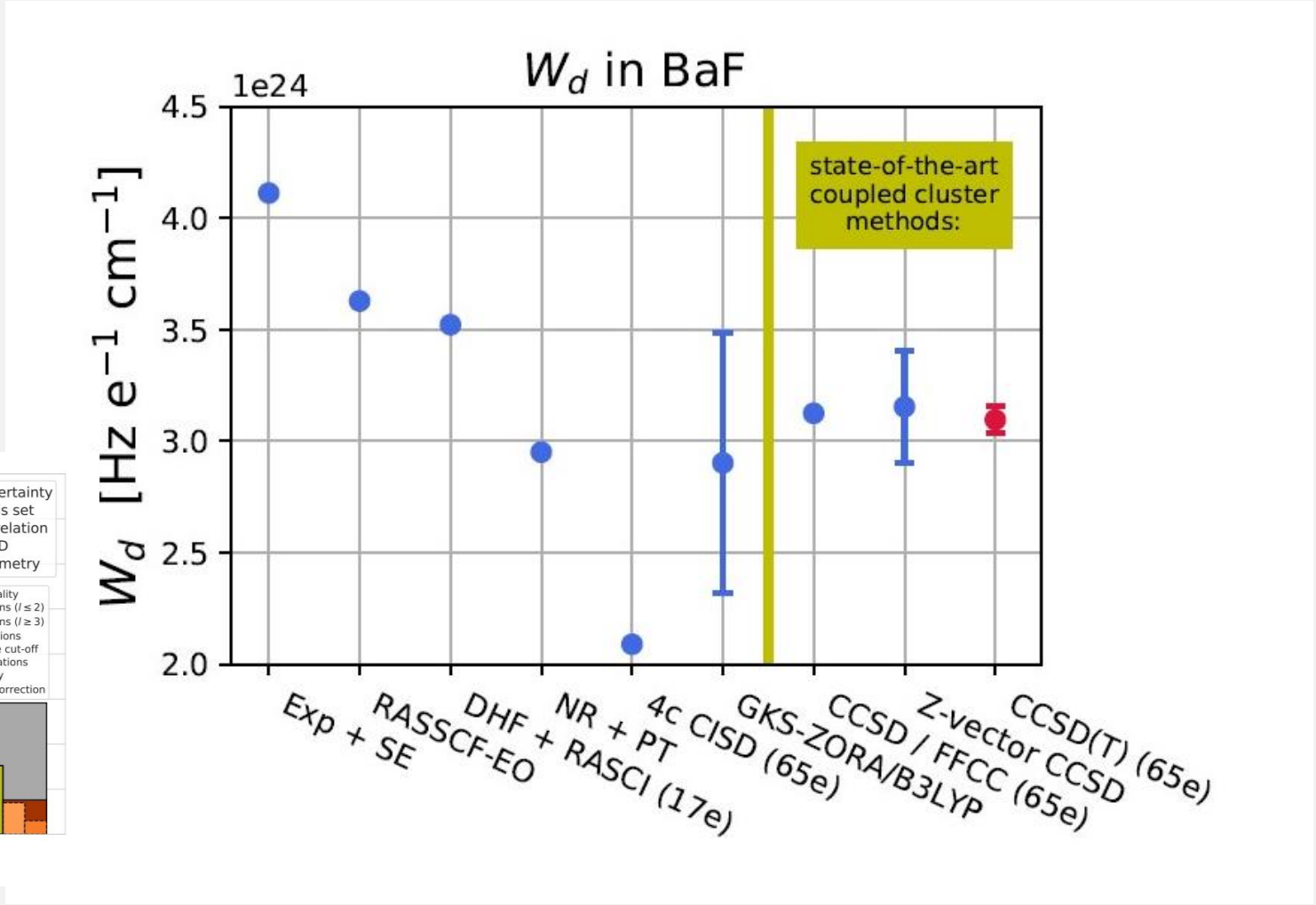
Interpreting the experiment

- Final recommended values:

BaF	W_d^* $[\frac{10^{24}\text{Hz}}{\text{e cm}}]$	W_s [Hz]
DC CCSD(T)	3.13 ± 0.24	8.29 ± 0.12

Pi Haase





Interpreting the experiment

- Final recom
-

BaF	W_d^* [
DC CCSD(T)	3.13

Pi Haase

The Journal of Chemical Physics

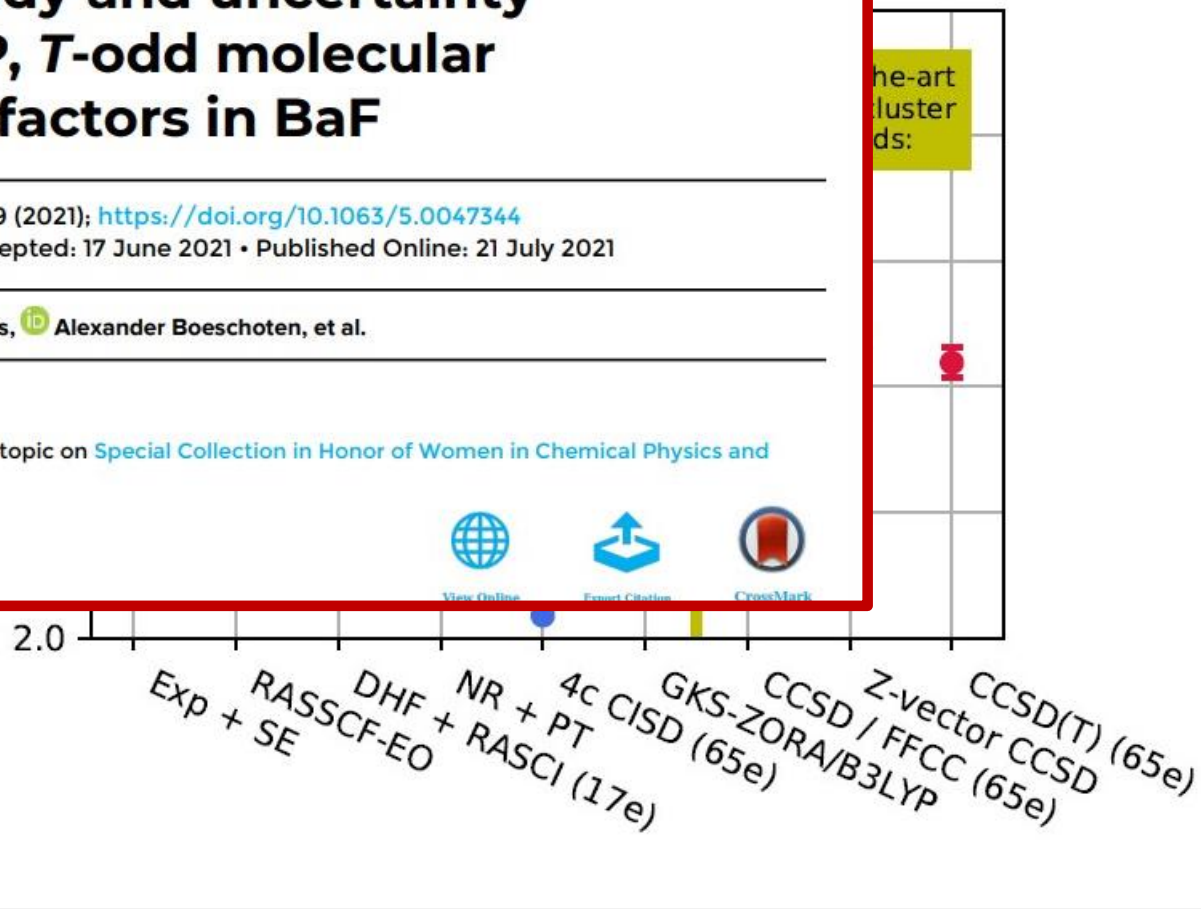
Systematic study and uncertainty evaluation of *P*, *T*-odd molecular enhancement factors in BaF

Cite as: J. Chem. Phys. **155**, 034309 (2021); https://doi.org/10.1063/5.0047344
Submitted: 12 February 2021 • Accepted: 17 June 2021 • Published Online: 21 July 2021

Pi A. B. Haase, Diewertje J. Doeglas, Alexander Boeschoten, et al.

COLLECTIONS

Paper published as part of the special topic on Special Collection in Honor of Women in Chemical Physics and Physical Chemistry



Interpreting the experiment

- Is the uncertainty estimate realistic?

How do we assign uncertainties?

- Calculate the same property in a lighter homologue (and compare to experiment)
- Calculate a different property in the same atom/molecule (and compare to experiment)
- Perform a computational investigation to assign uncertainties based on method incompleteness

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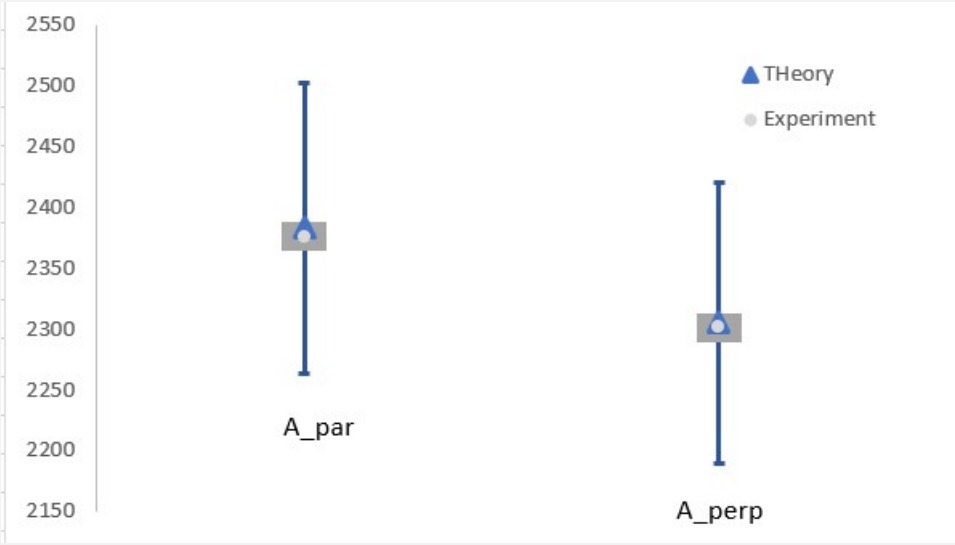
Interpreting the experiment

BaF	W_d^* $[\frac{10^{24}\text{Hz}}{\text{e cm}}]$	W_s [Hz]
DC CCSD(T)	3.13 ± 0.24	8.29 ± 0.12

- Is the uncertainty estimate realistic?
- Use a similar property, where comparison to experiment is possible, as a sanity check
- Magnetic hyperfine structure constants

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)	



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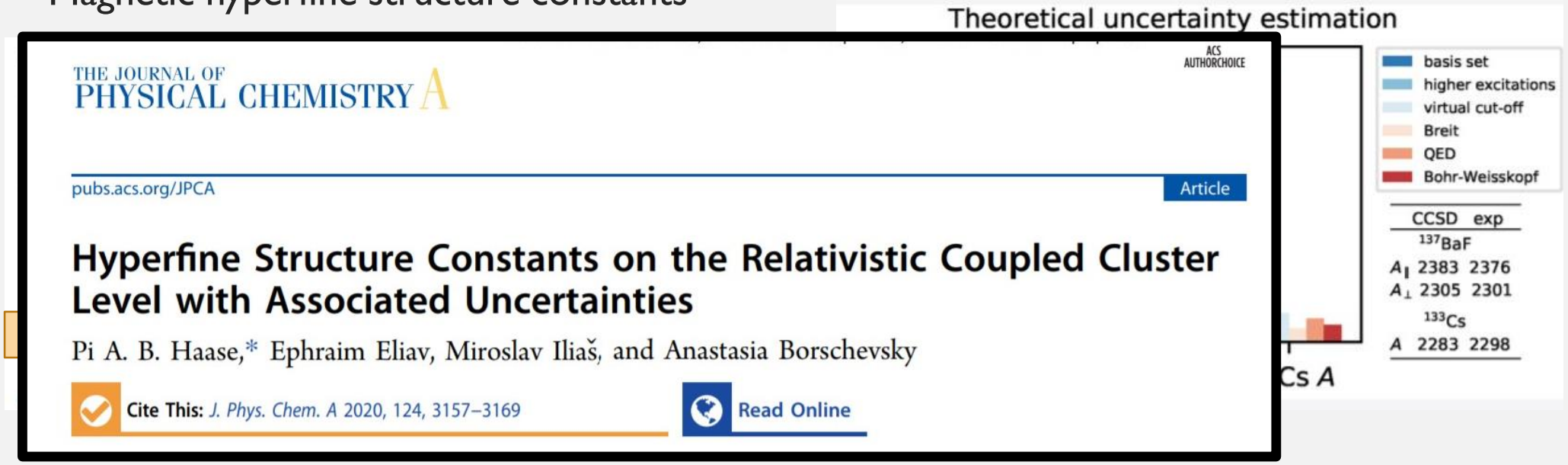
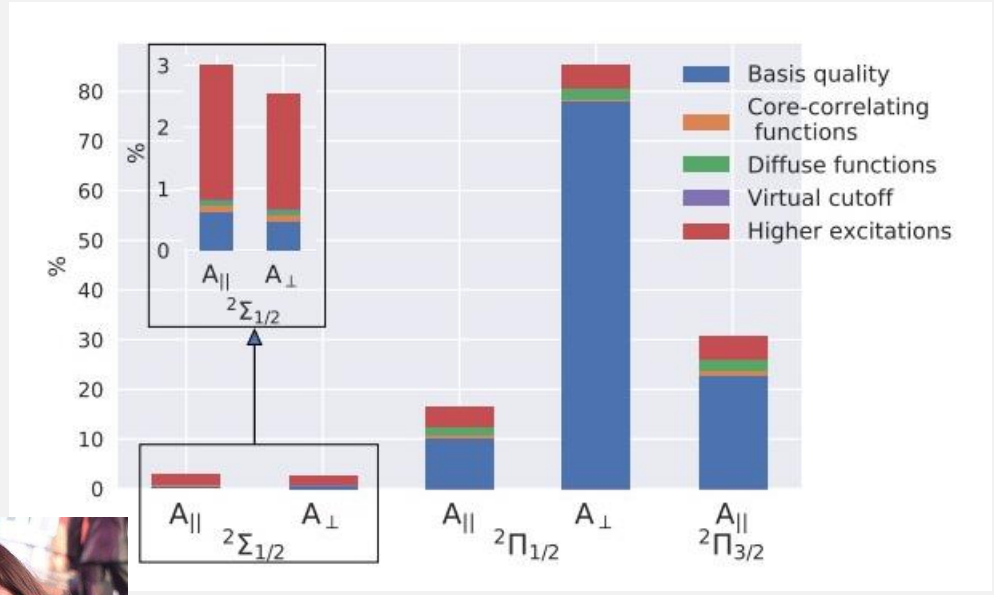


Hyperfine structure constants: predictive power

- Calculations of excited state HFS parameters in molecules are rare
- We looked at the F HFS coupling constant in the ground and excited states of BaF

State		Theory		Experiment
$^2\Sigma_{1/2}$	$A_\parallel$	CCSD(T)	71.22 ± 2.14	71.73 ± 0.09^a
	$A_\perp$	"	64.02 ± 1.62	63.51 ± 0.03^a
$^2\Pi_{1/2}$	$A_\parallel$	FSCC	51.97 ± 8.25	58.64 ± 0.27^b
	$A_\perp$	"	2.02 ± 1.51	3.58 ± 0.14^b
$^2\Pi_{3/2}$	$A_\parallel$	FSCC	13.40 ± 3.86	15.85 ± 0.09^b



Malika Denis

Pi Haase

Yuly Chamorro

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Benchmarking of the Fock-space coupled-cluster method and uncertainty estimation: Magnetic hyperfine interaction in the excited state of BaF

Malika Denis, Pi A. B. Haase, Maarten C. Mooij, Yuly Chamorro, Parul Aggarwal, Hendrick L. Bethlem, Alexander Boeschoten, Anastasia Borschevsky, Kevin Esajas, Yongliang Hao, Steven Hoekstra, Joost W. F. van Hofslot, Virginia R. Marshall, Thomas B. Meijknecht, Rob G. E. Timmermans, Anno Touwen, Wim Ubachs, Lorenz Willmann, and Yanning Yin (NL-*e*EDM Collaboration)

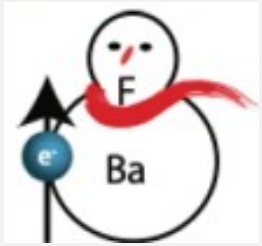
Phys. Rev. A **105**, 052811 – Published 31 May 2022

State		
$^2\Sigma_{1/2}$	$A_\parallel$	CCSD(
	$A_\perp$	"
$^2\Pi_{1/2}$	$A_\parallel$	FSCC
	$A_\perp$	"
$^2\Pi_{3/2}$	$A_\parallel$	FSCC

Malika Denis

Pi Haase

Yuly Chamorro

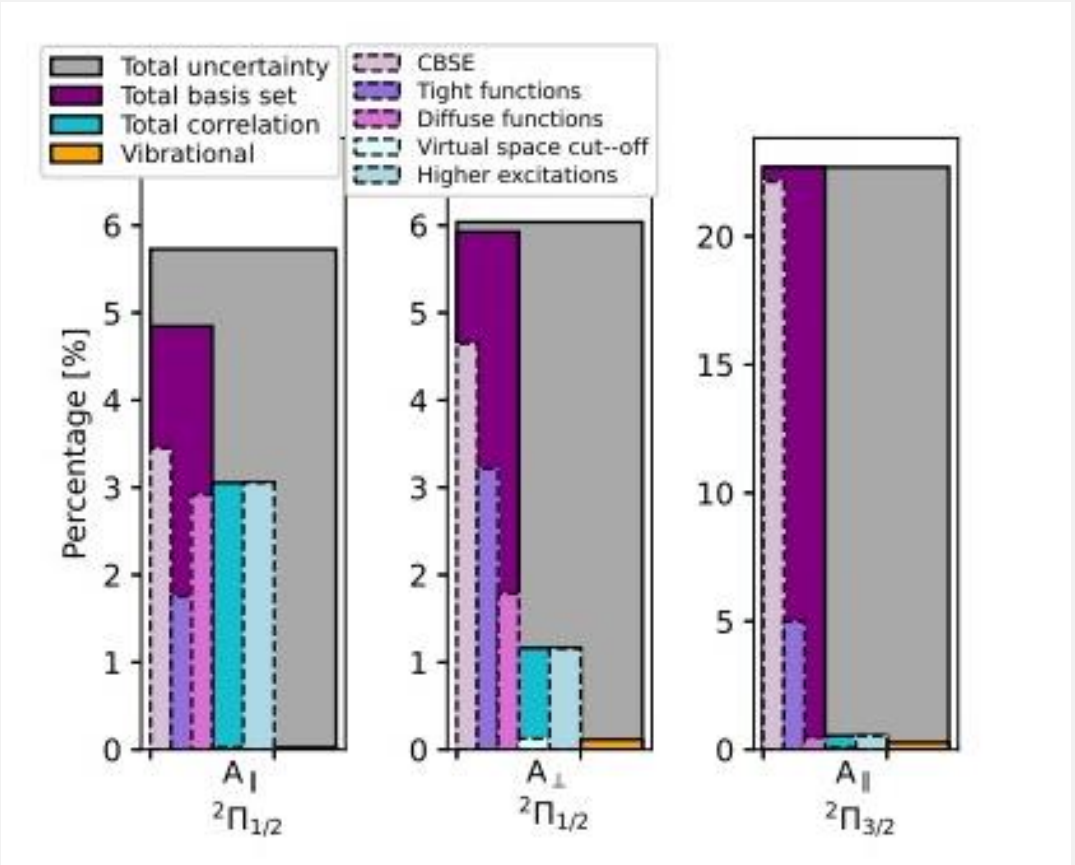


Hyperfine structure constants: predictive power

- Calculations of excited state HFS parameters in molecules are rare
- We looked at the ^{137}Ba HFS coupling constant in the excited states of BaF

	$^2\Pi_{1/2}$ $A_\parallel$	$A_\perp$	$^2\Pi_{3/2}$ $A_\parallel$
Baseline CBS(H)	394.5	242.8	36.6
Corrections			
Diffuse functions	-7.0	-7.7	-1.7
Tight functions	11.6	4.3	-0.2
Vibrational effects	-0.1	-0.3	-0.1
Final results	399.0 ± 22.9	239.1 ± 14.4	34.6 ± 7.9
Experiment	413.2 ± 0.6	254.3 ± 0.5	–

Yuly Chamorro



Tim Langen & Felix Kogel,
TU Vienna

OPEN ACCESS

Magnetic hyperfine structure constants of ^{137}BaF in the $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ excited states

Yuly Chamorro [1,*], Felix Kogel [2], Tim Langen [2,3], and Anastasia Borschevsky [1]

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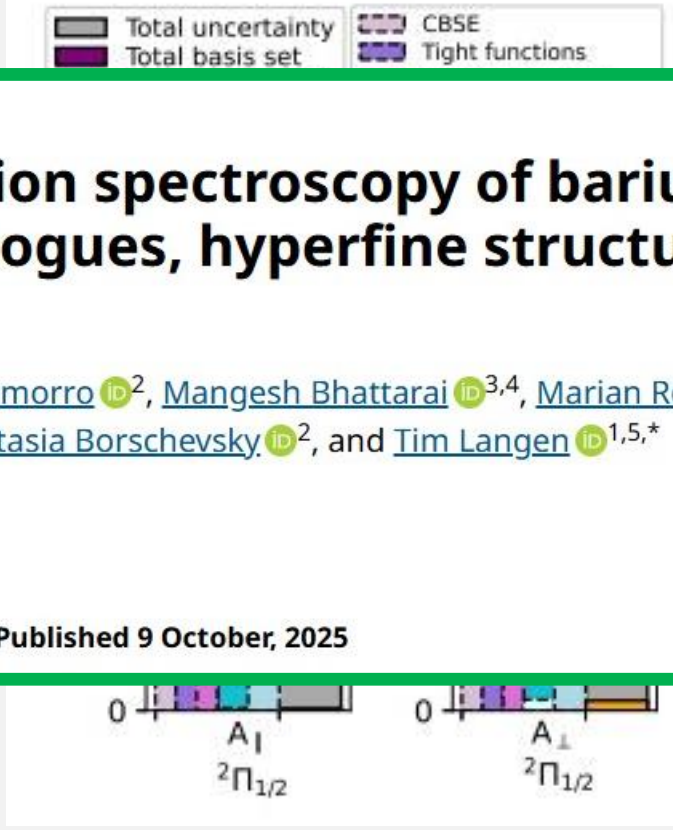
Phys. Rev. A **112**, 042808 – **Published 9 October, 2025**

	$^2\Pi_{1/2}$ $A_\parallel$	$^2\Pi_{1/2}$ $A_\perp$	$^2\Pi_{3/2}$ $A_\parallel$
Tight functions	11.6		
Vibrational effects	-0.1		
Final results	399.0 ± 22.9	239.1 ±	
Experiment	413.2 ± 0.6	254.3 ±	

Yuly Chamorro



OPEN ACCESS

High-resolution spectroscopy of barium monofluoride: Odd isotopologues, hyperfine structure, and isotope shifts

Felix Kogel [1], Yuly Chamorro [2], Mangesh Bhattarai [3,4], Marian Rockenhäuser [1,5], Tatsam Garg [1,5], David DeMille [3,4,6], Anastasia Borschevsky [2], and Tim Langen [1,5,*]

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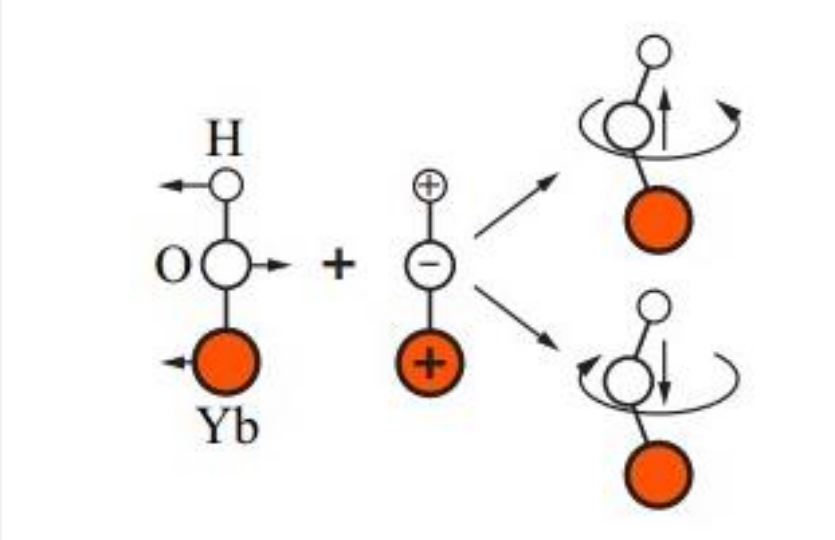
Phys. Rev. A **112**, 042807 – **Published 9 October, 2025**

APPLICATIONS

- Ionization potentials of CaF, SrF, BaF, and RaF: meV accuracy, uncertainty estimation, and predictive power
- P,T-violating coupling constants and molecular parameters
  - Search for the electric dipole moment on the electron: the NL-eEDM collaboration
  - Triatomic molecules: BaOH and YbOH

TRIATOMIC MOLECULES

- Polyatomic molecules emerge as good candidates for eEDM experiments due to the long-lived close-lying opposite parity eigenstates
- **BaOH** and YbOH are also expected to be laser-coolable
- What about sensitivity to BSM physics?



- Polyatomic molecules emerge as good candidates for eEDM experiments due to the long-lived close-lying opposite parity eigenstates (*l*-doublets)
- BaOH and YbOH are also expected to be laser-coolable
- What about sensitivity to BSM physics?
- Sensitivity to eEDM and to *P,T*-violating nuclear magnetic quadrupole moment (NMQM) found to be similar to that of diatomic homologues

	W_d [10^{24}Hz/(e·cm)]	W_M [10^{23}Hz/(e·cm^2)]
BaF	3.13	-0.385
BaOH	3.21	-0.392
YbF	23.37	-1.055
YbOH	23.56	-1.067

Malika Denis

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- Sensitivity to eEDM and to *P,T*-violating nuclear magnetic quadrupole moment (NMQM) found to be similar to that of diatomic homologues
- Accuracy test: HFS constants:

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TABLE VII. The $A_\parallel$ 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 $A_\parallel$	Expt. $A_\parallel$	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		

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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

Enhancement factor for the electric dipole moment of the electron in the BaOH and YbOH molecules

Malika Denis[1,*], Pi A. B. Haase[1], Rob G. E. Timmermans[1], Ephraim Eliav[2], Nicholas R. Hutzler[3], and Anastasia Borschevsky[1]

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Phys. Rev. A **99**, 042512 – **Published 19 April, 2019**

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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)]

- Polyato
  lived close-lying opposite parity eigenstates (*l*-doublets)
- BaOH and Y
- What abou
- Sensitivity
  calculated a
- Accuracy te

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	$A_{\parallel}$[a]	6979 (35)	7174.9			
^{171}YbOH	$A_{\perp}$[b]	6745(15)				
^{173}YbOH	$A_{\parallel}$	-1929(11)	−1976.3	-1600	-1300	
^{173}YbOH	$A_{\perp}$	-1856 (5)		-1600		
^{173}YbOH	e^2Qq_0	-3319 (48)	−3502			-3492

	W_d [10^{24}Hz/(e·cm)]	W_M [10^{23}Hz/(e·cm^2)]
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- Static and dynamic polarizability in BaOH
- Important in the context of trapping

	$\alpha_{\parallel}$ (a.u.)	α_{+}(a.u.)
Static	200.8(24)	297(5)
Dynamic (λ=1064nm)	357(31)	714(29)

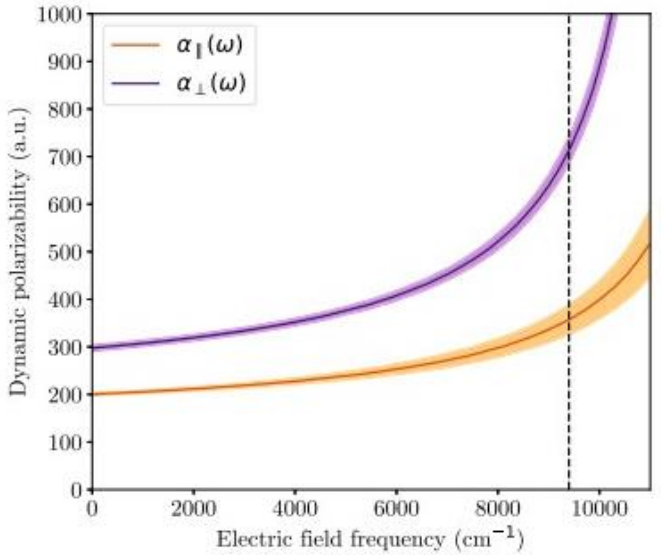

FIG. 2. Parallel and perpendicular components of the dynamic polarizability (solid lines) with uncertainty bounds (shaded regions) as a function of the frequency of the external electric field. The dashed line corresponds to the 1064-nm laser.

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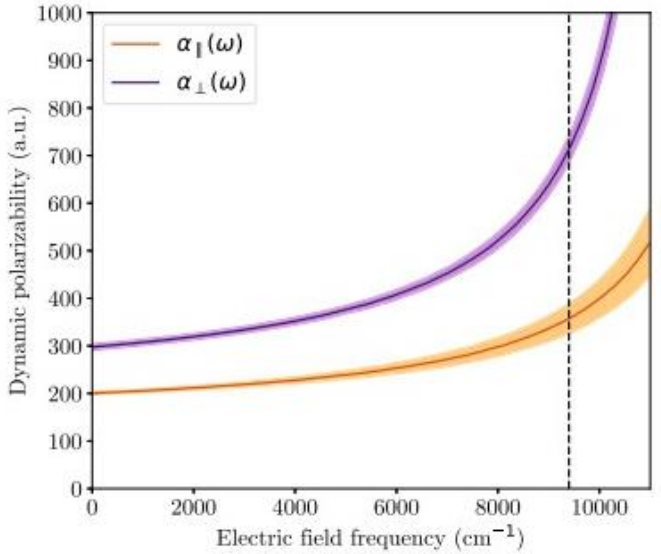
Eifion Prinsen

Agustin Aucar

Lukas Pasteka



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- Stati
- Impe

PHYSICAL REVIEW A **113**, 022809 (2026)

***Ab initio* calculations of the static and dynamic polarizability of BaOH**

Eifion H. Prinsen,[1,2] Anastasia Borschevsky,[1,2] Steven Hoekstra,[1,2] Achintya K. Dutta,[3] Sudipta Chakraborty,[3] Bart J. Schellenberg,[1,2] Lukáš F. Pašteka,[1,2,4,*] and I. Agustín Aucar[1,2,5,†]

[1]*Van Swinderen Institute for Particle Physics and Gravity, University of Groningen, The Netherlands*
[2]*Nikhef, National Institute for Subatomic Physics, Amsterdam, The Netherlands*
[3]*Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India*
[4]*Department of Physical and Theoretical Chemistry, Comenius University, Bratislava, Slovakia*
[5]*Instituto de Modelado e Innovación Tecnológica, Facultad de Ciencias Exactas y Naturales y Agrimensura, Universidad Nacional del Nordeste, Corrientes, Argentina*

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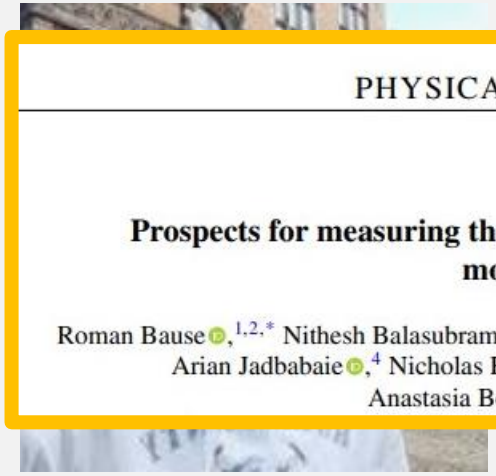
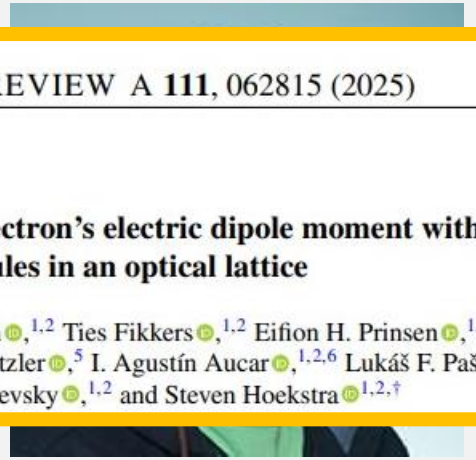
Eifion Prinsen



Agustin Aucar



Lukas Pasteka

PHYSICAL REVIEW A **111**, 062815 (2025)

Prospects for measuring the electron's electric dipole moment with polyatomic molecules in an optical lattice

Roman Bause,[1,2,*] Nithesh Balasubramanian,[1,2] Ties Fikkers,[1,2] Eifion H. Prinsen,[1,2] Kees Steinebach,[3] Arian Jadbabaie,[4] Nicholas R. Hutzler,[5] I. Agustín Aucar,[1,2,6] Lukáš F. Pašteka,[1,2,7] Anastasia Borschevsky,[1,2] and Steven Hoekstra[1,2,†]

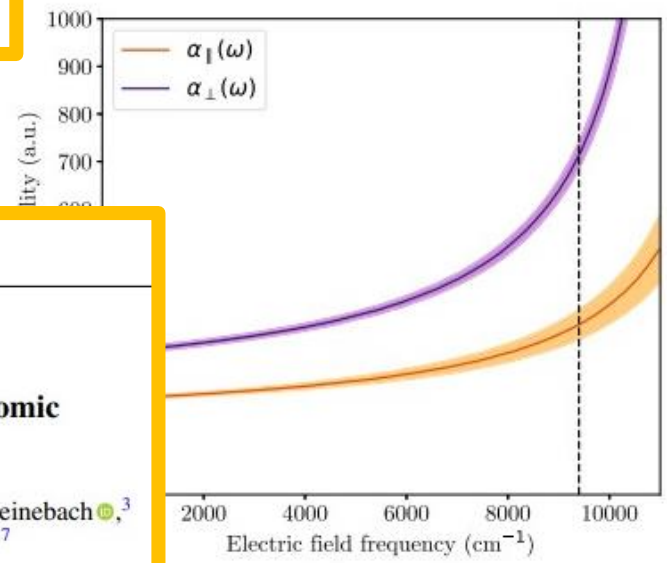


FIG. 2. Parallel and perpendicular components of the dynamic polarizability (solid lines) with uncertainty bounds (shaded regions) as a function of the frequency of the external electric field. The dashed line corresponds to the 1064-nm laser.

- Stati
- Impe

PHYSICAL REVIEW A **113**, 022809 (2026)

***Ab initio* calculations of the static and dynamic polarizability of BaOH**

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[1]*Van Swinderen Institute for Particle Physics and Gravity, University of Groningen, The Netherlands*

See talk by Steven Hoekstra, Thursday morning:

09:45 → 10:15 **Precision measurements to test fundamental physics using trapped molecules**

Speaker: Steven Hoekstra (University of Groningen, and Nikhef)

PHYSICAL REVIEW A **111**, 062815 (2025)

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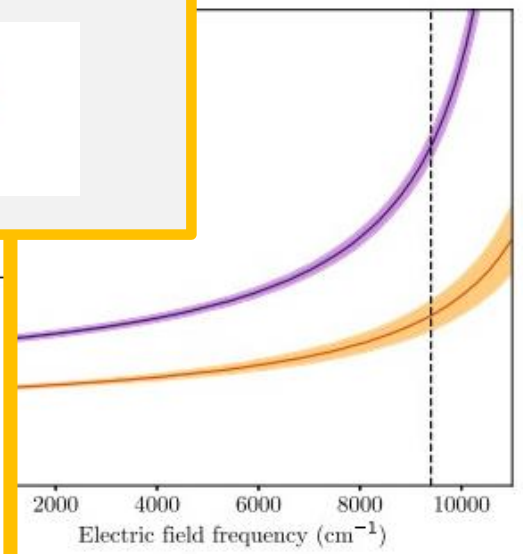

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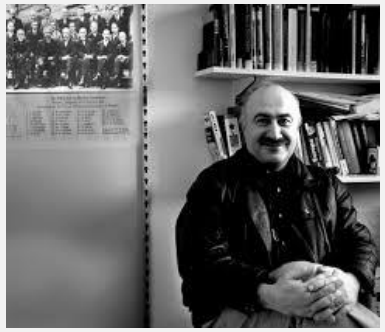
CONCLUSIONS

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



Ephraim Eliav

Miroslav Ilias

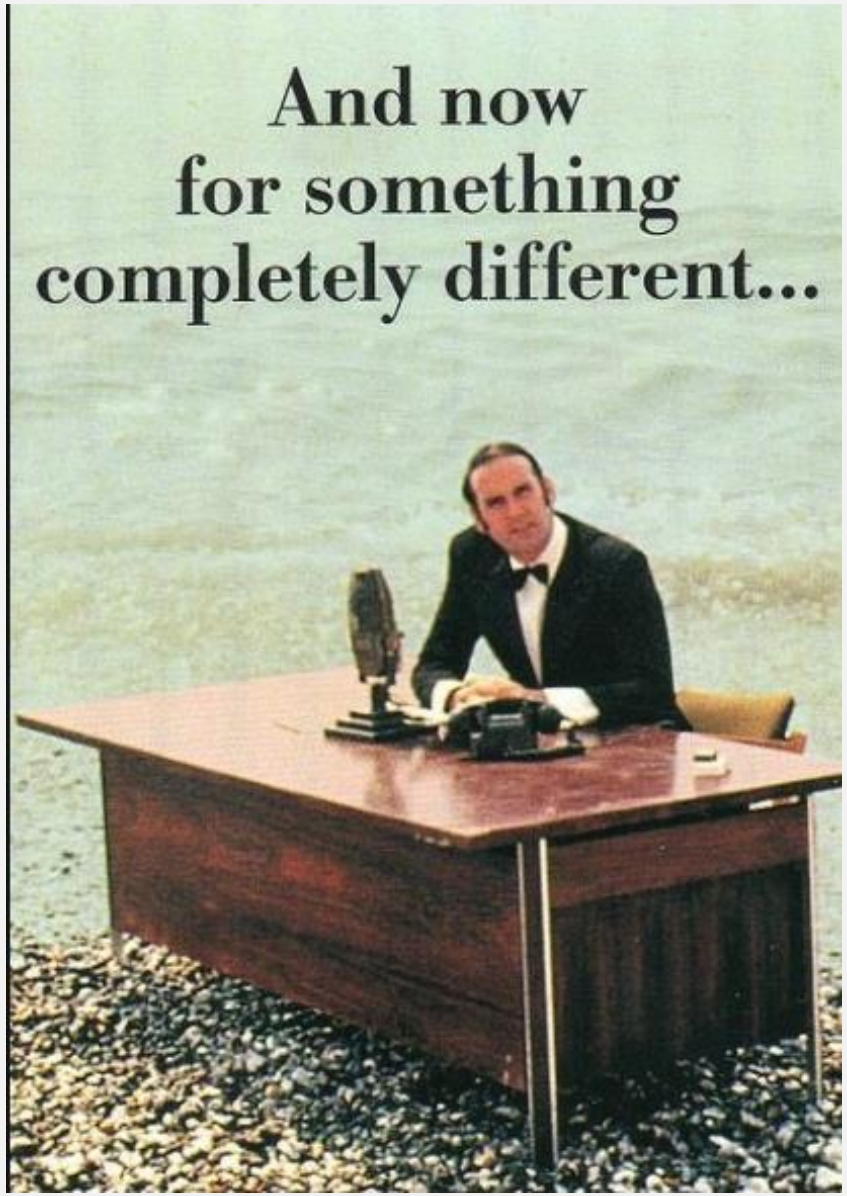
Peter Schwerdtfeger

Jacinda Ginges

Victor Flambaum

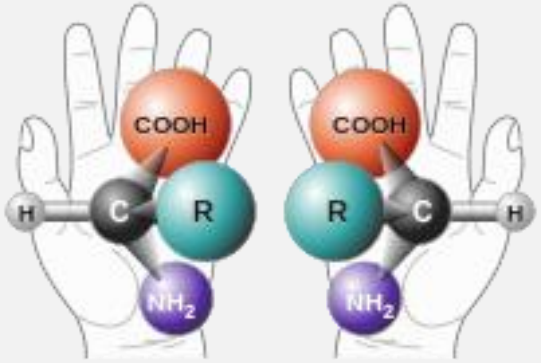
Lukas Pasteka

Konstantin Gaul


And now
for something
completely different...

PARITY VIOLATION IN CHIRAL MOLECULES

- **Is there a difference in the properties of the right- and the left handed enantiomers?**



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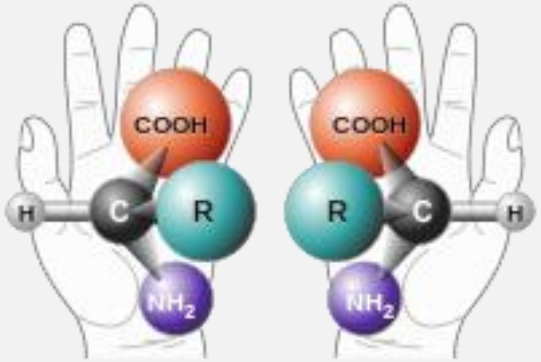
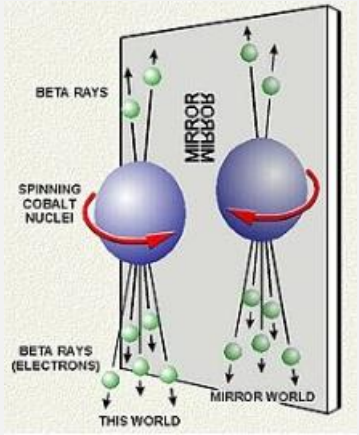
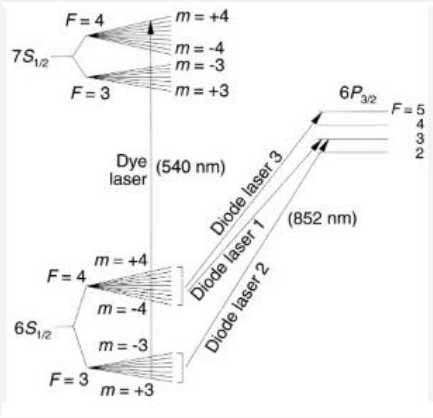


- PV is firmly established in nuclear and atomic physics
-



Decay of ^{60}Co



Forbidden 6s-7s transition in atomic Cs

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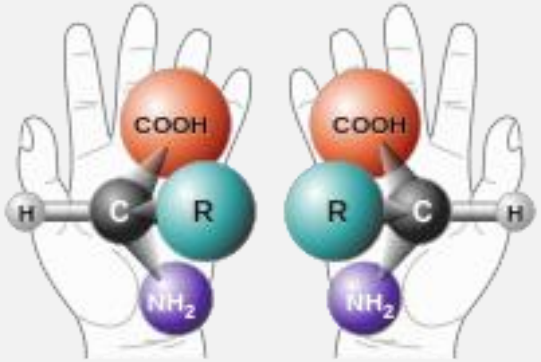
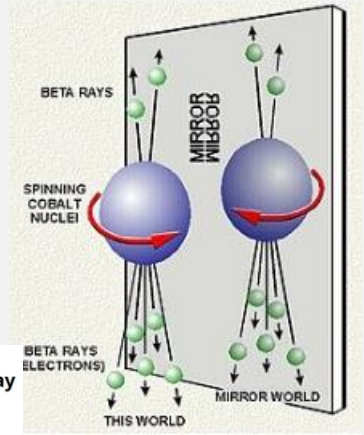


No longer measuring zero!

- PV is firmly established in nuclear and atomic physics
-

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Experimental Test of Parity Conservation in Beta Decay

C. S. Wu

E. Ambler, R. W. Hayward, D. D. Hoppes, and R. P. Hudson

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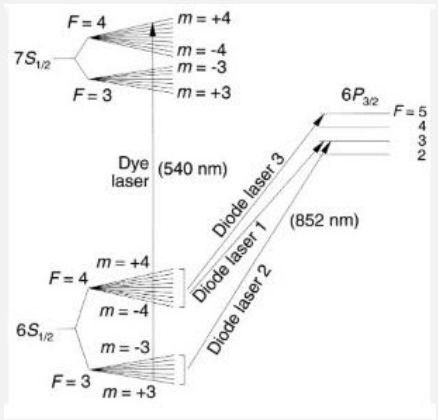
Phys. Rev. **105**, 1413 – **Published 15 February, 1957**

Decay of ^{60}Co



Forbidden 6s-7s transition in atomic Cs


Science

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HOME > SCIENCE > VOL. 275, NO. 5307 > MEASUREMENT OF PARITY NONCONSERVATION AND AN ANAPOLE MOMENT IN CESIUM

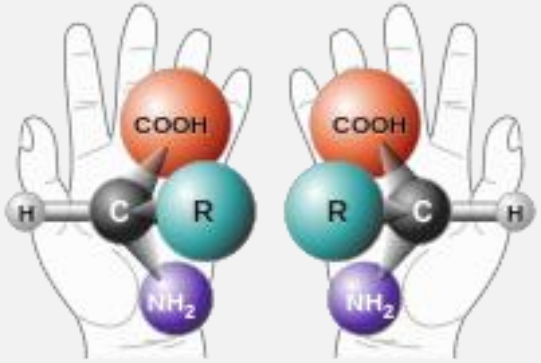
RESEARCH ARTICLES

Measurement of Parity Nonconservation and an Anapole Moment in Cesium

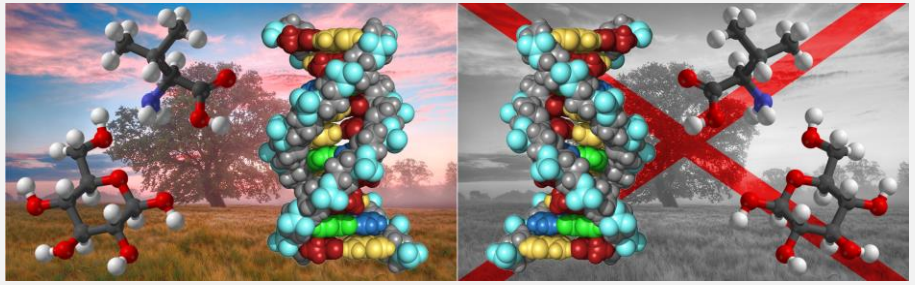
C. S. WOOD, S. C. BENNETT, D. CHO, B. P. MASTERSON, J. L. ROBERTS, C. E. TANNER, AND C. E. WIEMAN Authors Info & Affiliations

SCIENCE · 21 Mar 1997 · Vol 275, Issue 5307 · pp. 1759-1763 · DOI: 10.1126/science.275.5307.1759

- **Is there a difference in the properties of the right- and the left handed enantiomers?**



- PV is firmly established in nuclear and atomic physics
- In chiral molecules, the weak neutral current between the electrons and the nuclei is predicted to result in a tiny energy difference between the enantiomers.
- If detected, this could
  - Constitute a test of the SM
  - Help explain the origins of biohomochirality
  - Allow deeper understanding of electronic structure effects



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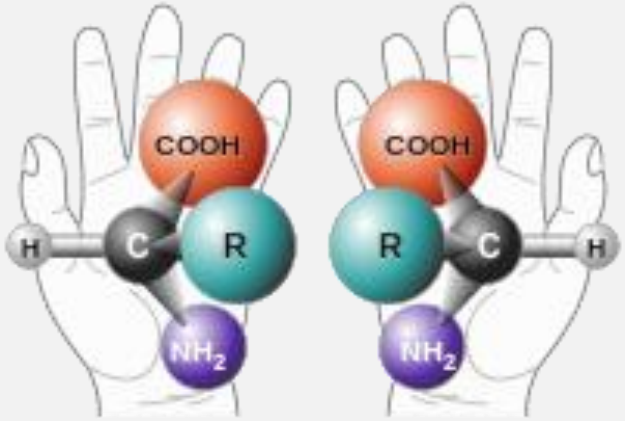
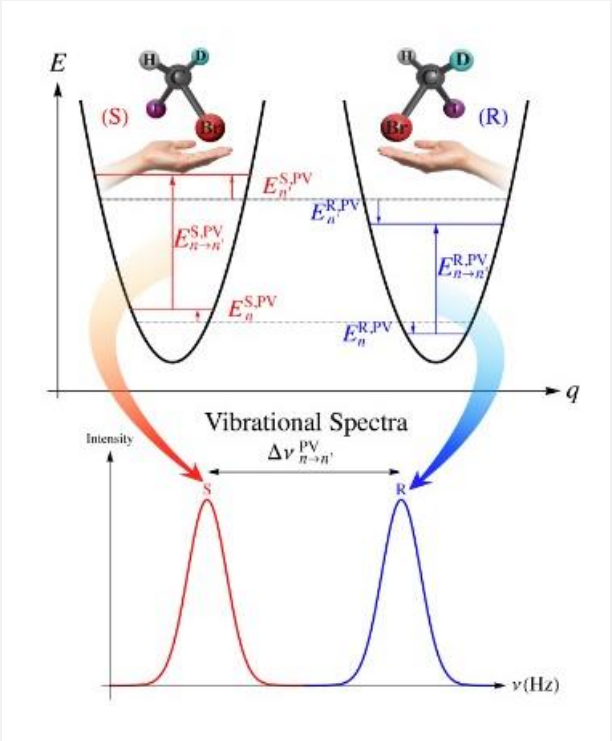


- So far, no detection!
- The search continues: in electronic transitions, NMR spectroscopy, and in **vibrational spectroscopy**

- **Search for parity violation in vibrational spectroscopy.**

$$E_n^{\mathrm{PV}} = \langle n | V^{\mathrm{PV}}(q) | n \rangle$$

$$\Delta\nu_{m\to n}^{\mathrm{PV}} = \frac{2}{h}(E_n^{\mathrm{PV}} - E_m^{\mathrm{PV}})$$



- Measure $h\nu_L$-$h\nu_R$
- Measurements performed at Laboratoire Physique des Lasers (LPL), on the C-F stretch vibration in CHFClBr

- **Search for parity violation in vibrational spectroscopy.**

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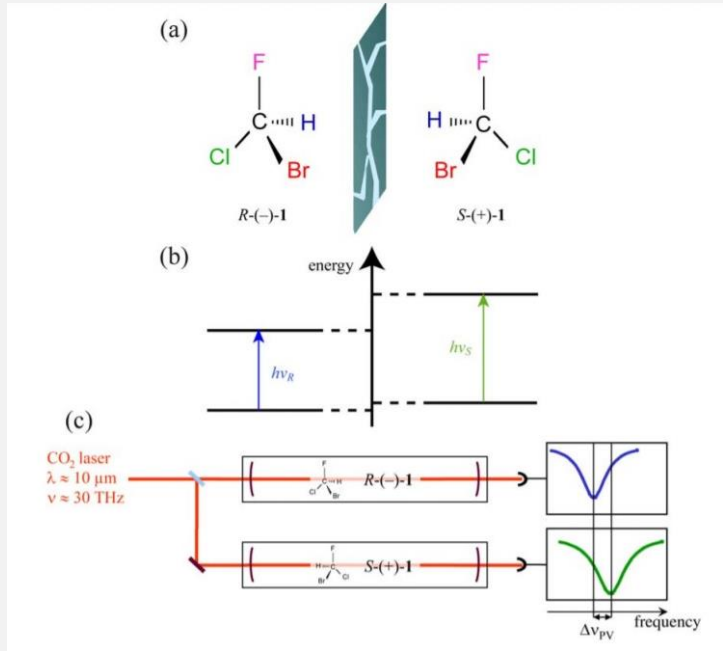
- Upper limit of $\frac{\Delta\nu_{PV}}{\nu} = 2.5 \times 10^{-13}$



Progress toward the first observation of parity violation in chiral molecules by high-resolution laser spectroscopy†

Benoît Darquié, Clara Stoeffler, Alexander Shelkovnikov, Christophe Daussy, Anne Amy-Klein, Christian Chardonnet, Samia Zrig, Laure Guy, Jeanne Crassous ... See all authors

First published: 13 September 2010 | https://doi.org/10.1002/chir.20911 | Citations: 95

18 C. Daussy, T. Marrel, A. Amy-Klein, C. Nguyen, C. J. Bordé and C. Chardonnet, *Physical Review Letters*, 1999, **83**, 1554.

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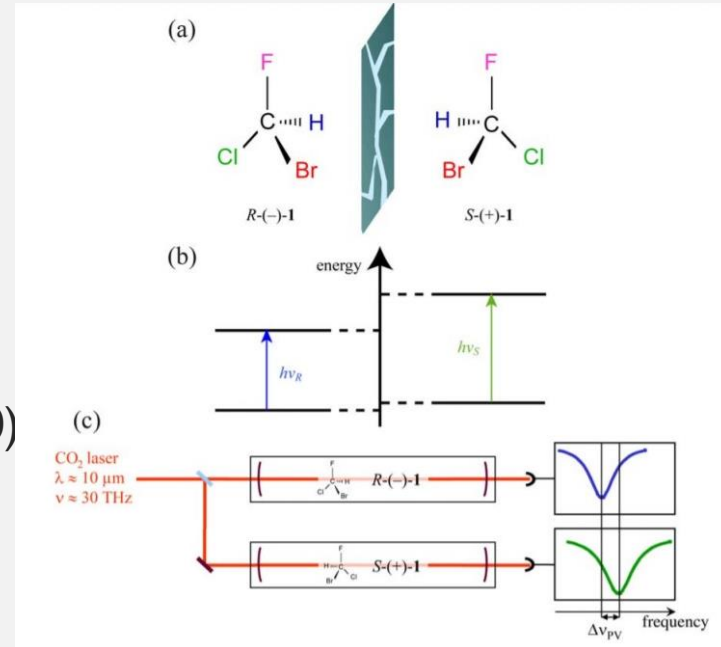
- Upper limit of $\frac{\Delta\nu_{PV}}{\nu} = 2.5 \times 10^{-13}$
- Theoretical estimates of the effect ~10^{-17}

(Phys. Rev. Lett. **84**, 3807 (2000); Phys. Rev. A **71**, 012103 (2005);

Phys. Rev. A **103**, 042819 (2021); Phys. Rev. Lett. **125**, 123004 (2020)



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- Better candidate molecule needed!
- Shopping list:
  - Stable, commercially available
  - Can be separated into pure enantiomers
  - Can be brought into the gas phase
  - Should contain heavy elements (absolute PV energy predicted to scale as Z^5)
  - Should have strong vibrational transitions in the range of the lasers (4-15 μm)
- Relative effects of the order 10^{-15} can now be detected at LPL

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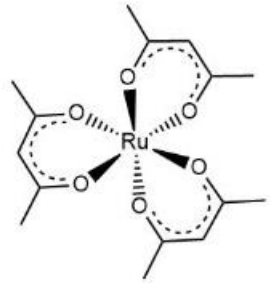

Fig. 1 Chemical structure of Δ-Ru(acac)$_3$

43. Darquié, B.; Saleh, N.; Tokunaga, S. K.; Srebro-Hooper, M.; Ponzi, A.; Autschbach, J.; Decleva, P.; Garcia, G. A.; Crassous, J.; Nahon, L. Valence-shell photoelectron circular dichroism ruthenium(III)-tris-(acetylacetonato) gas-phase enantiomers. *Phys. Chem. Chem. Phys.* **2021**, *23*, 24140– 24153, DOI:

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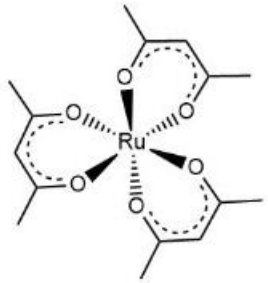

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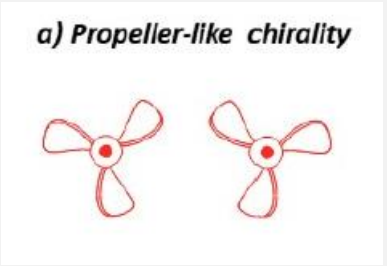

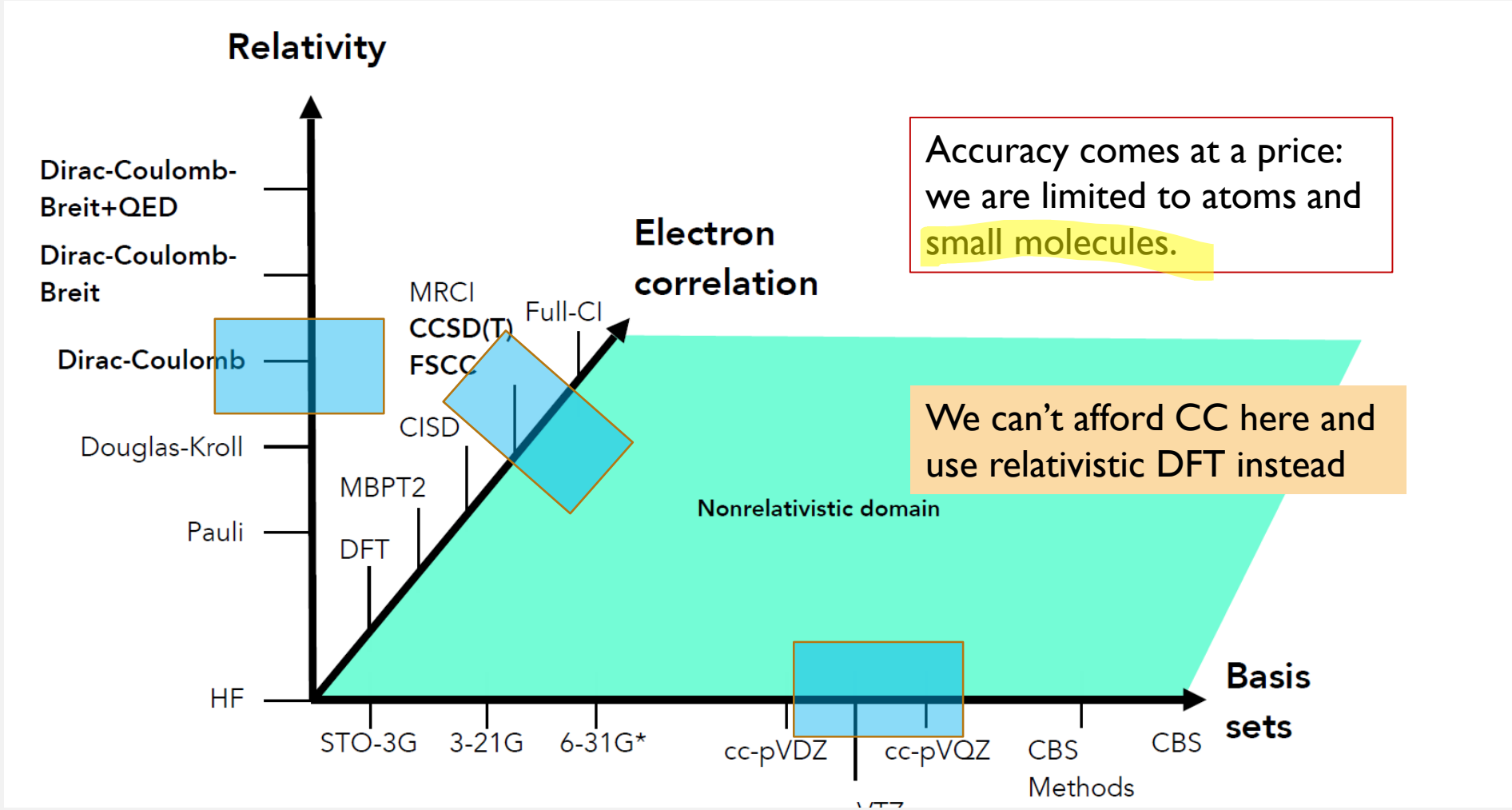
Relativity
Dirac-Coulomb-Breit+QED
Dirac-Coulomb-Breit
Dirac-Coulomb
Douglas-Kroll
Pauli
HF
Electron correlation
MRCI
CCSD(T)
FSCC
Full-CI
CISD
MBPT2
DFT
Nonrelativistic domain
STO-3G
3-21G
6-31G*
cc-pVDZ
cc-pVQZ
CBS
Methods
CBS
Basis sets
Accuracy comes at a price: we are limited to atoms and small molecules.
We can't afford CC here and use relativistic DFT instead

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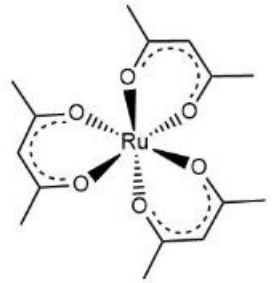

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mode no.	ν(cm^{-1})	IR int.(KM/mol)	$\Delta\nu_{PV}$ (mHz)	$\lvert\Delta\nu_{PV}/\nu\rvert$
17	182.0	0.009	-448.7	7.22E-14
19	200.8	1.718	-297.9	4.57E-14
20	222.9	0.065	279.2	3.80E-14
29	327.2	7.884	325.3	3.40E-14
52	952.6	9.564	-30.4	1.04E-15
53	953.7	1.793	-33.0	1.13E-15
100	1586.0	453.5	-83.0	1.70E-15
102	1612.3	44.22	-110.9	2.25E-15

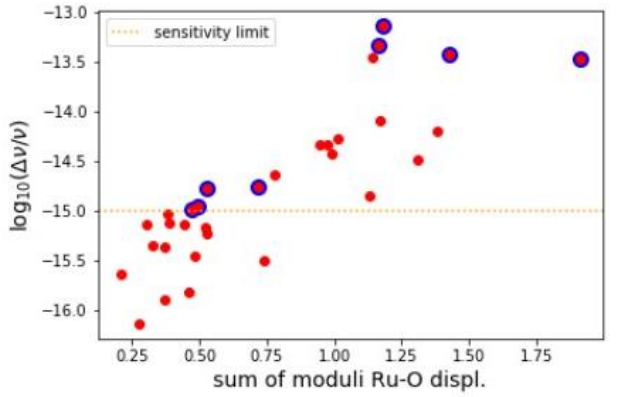

Fig. 3 Plot of all calculated relative parity violating frequency shifts ($\Delta\nu_{PV}/\nu$) of several vibrational transitions in Ru(acac)$_3$ as a function of the indicator (sum of moduli of Ru-O displacement, see text). The larger dots highlighted in blue correspond to the modes shown in Table 1, and

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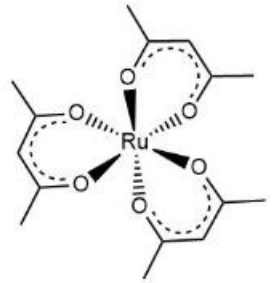

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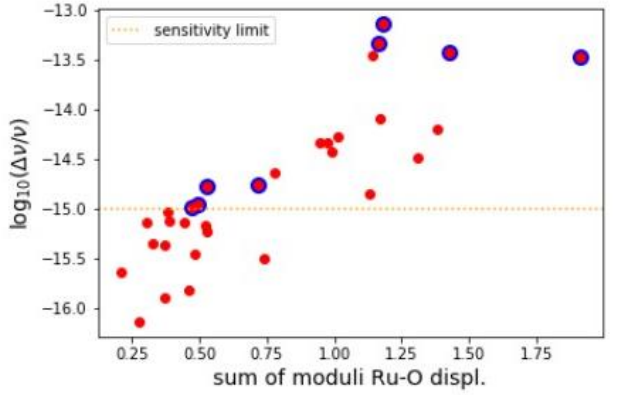

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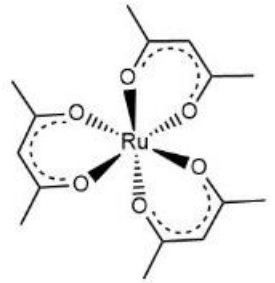

Fig. 1 Chemical structure of Δ-$Ru(acac)_3$

mode Os	corresp. mode Ru	overlap	ν_{PV}(Os) (Hz)	ν_{PV}(Os)/ν_{PV}(Ru)	ν (cm^{-1})	IR int.(KM/mol)	$\lvert\Delta\nu/\nu\rvert$
16	17	0.996	-9.72	21.7	191.4	0.091	1.51E-12
19	19	0.961	-9.59	32.2	210.9	2.356	1.44E-12
20	20	0.948	4.30	15.4	224.2	0.013	5.86E-13
29	29	0.838	3.09	9.5	307.6	2.392	3.39E-13
52	52	0.830	-1.47	48.4	952.2	0.464	5.00E-14
53	53	0.831	-1.32	40.1	954.0	1.272	4.48E-14
100	100	0.955	-1.04	12.7	1562.5	245.6	2.16E-14
102	102	0.985	-0.31	3.6	1589.2	102.2	6.29E-15

Table 2 The PV shift of vibrational modes in $Os(acac)_3$ and a comparison to $Ru(acac)_3$. Modes in the two compounds were matched to each other according to their overlap as defined in section 3.

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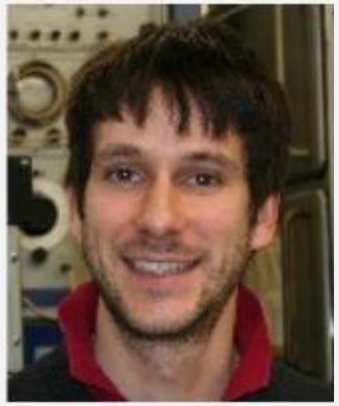
Marit Fiechter (now ETH Zurich)

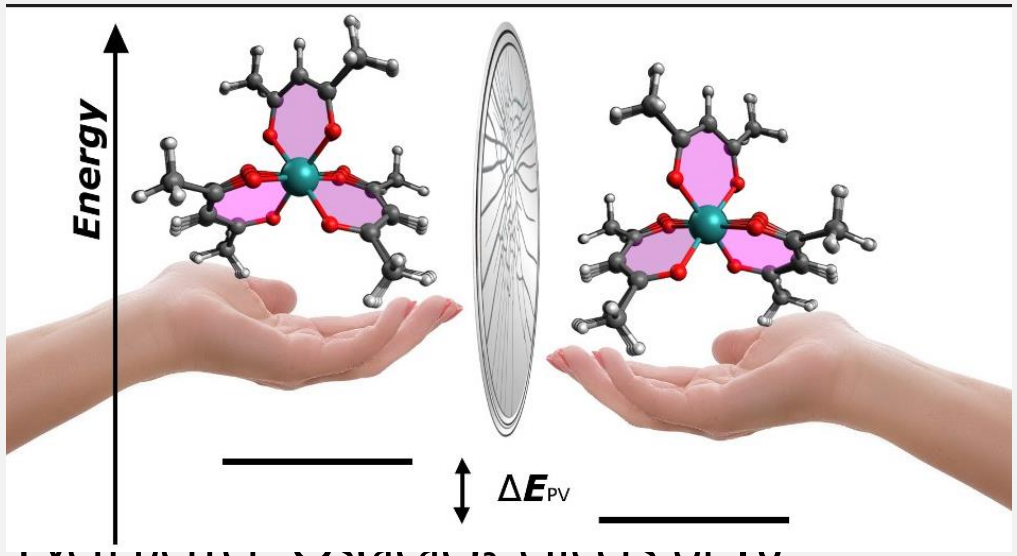


Benoît Darquié, LPL

Jeanne Crassous, Rennes

Pi Haase

Lukas Pasteka, Bratislava



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- Even better : $Os(acac)_3$, effects of 1%
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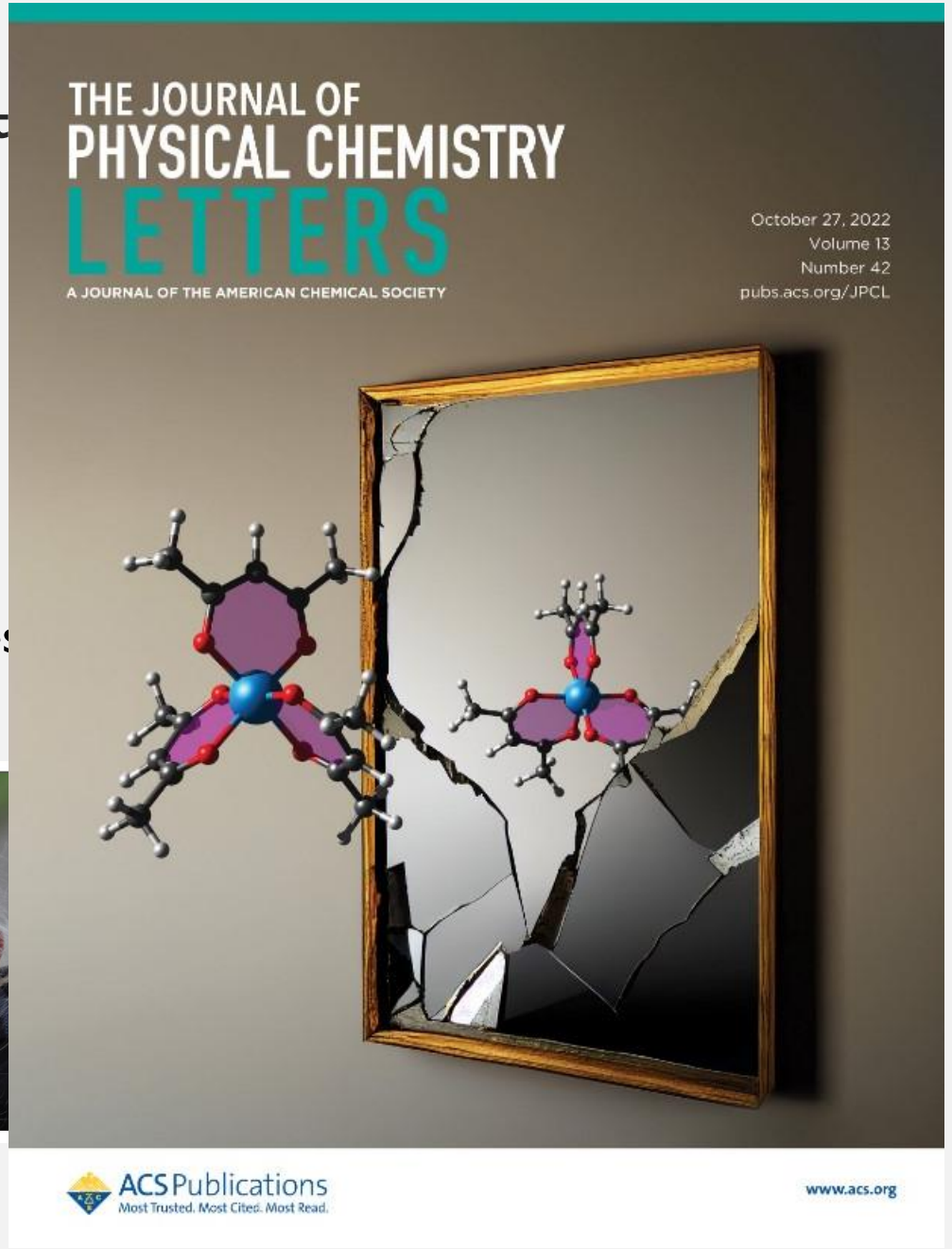

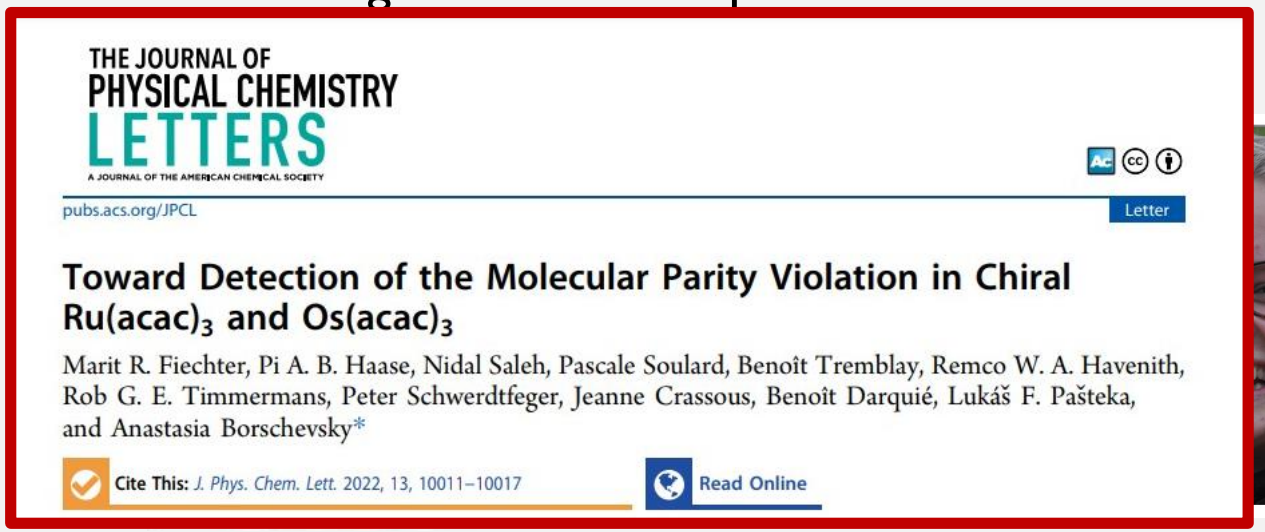
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Letter

Toward Detection of the Molecular Parity Violation in Chiral $Ru(acac)_3$ and $Os(acac)_3$

Marit R. Fiechter, Pi A. B. Haase, Nidal Saleh, Pascale Soulard, Benoît Tremblay, Remco W. A. Havenith, Rob G. E. Timmermans, Peter Schwerdtfeger, Jeanne Crassous, Benoît Darquié, Lukáš F. Pašteka, and Anastasia Borschevsky*

Cite This: *J. Phys. Chem. Lett.* 2022, 13, 10011−10017

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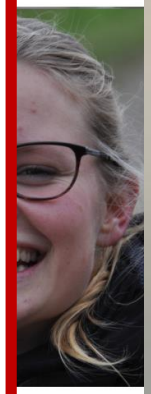

Benoît Darquié, LPL Jeanne Crassous, Rennes Pi Haase

- **Other fun candidates:**

- From simple:
- $CHDBrI^+$

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Cite this: *Chem. Commun.*, 2023, 59, 14579

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DOI: 10.1039/d3cc03787h

Large vibrationally induced parity violation effects in $CHDBrI^+$†

Eduardus,[a] Yuval Shagam,[b] Arie Landau,[b] Shirin Faraji,[c] Peter Schwerdtfeger,[d] Anastasia Borschevsky[a] and Lukáš F. Pašteka*[ae]

RESEARCH ARTICLE | SEPTEMBER 19 2023

Chiral molecule candidates for trapped ion spectroscopy by *ab initio* calculations: From state preparation to parity violation

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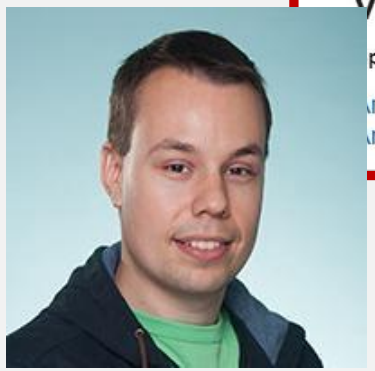
rie Landau ; Eduardus ; Doron Behar ; Eliana Ruth Wallach ; Lukáš F. Pašteka ; Shirin Faraji ; nastasia Borschevsky ; Yuval Shagam

Eduardus

Yuval Shagam, Technion



Lukas Pasteka, Bratislava

- **Other fun candidates:**

arXiv > physics > arXiv:2509.26407v1

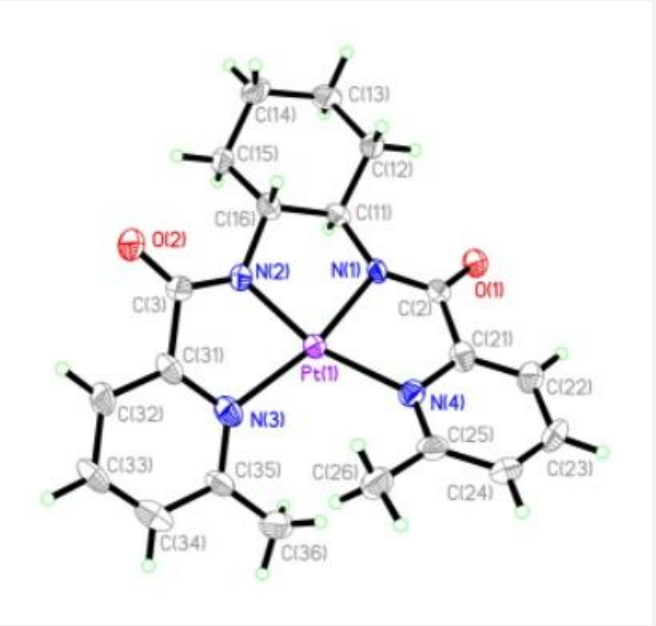
Physics > Chemical Physics

[Submitted on 30 Sep 2025]

Chiral Pt(Me-BPCH): Synthesis and theoretical investigation of parity violation sensitivity

Eduardus, J. Wietze J. van Boven, Charles Silva, Philip Karageorghis, D. Scott Bohle, Benoît Darquié, Anastasia Borschevsky, Lukáš F. Pašteka

- To complex:
- Pt(Me-BPCH)



Eduardus

Scott Bohle, McGill

Lukas Pasteka, Bratislava