Rigorous Relativistic Methods for Addressing $\mathcal{P}$- and $\mathcal{T}$-Nonconservation in Heavy-Element Molecules

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Overview

1. **Principles of relativistic molecular electronic-structure theory**

2. **Implementation of $\mathcal{P}$- and $\mathcal{T}$-non-conserving operators**

3. **Electron EDM interaction constant in HfF^+**

4. **Outlook: Other systems, other effects, new methods**

1. Four-Component Electronic-Structure Theory

Some Essentials

- Atomic basis sets; in low-energy approximation

  $\psi^S(\vec{r}) \approx \frac{\sigma \cdot \mathbf{p}}{m_0 c} \psi^L(\vec{r})$

  Kinetic-balance condition

- Solution of the Dirac-Coulomb Hartree-Fock equations

$$\begin{pmatrix} \left(\hat{V}_{\rm nuc} + \hat{v}_{\rm DCHF}\right) \mathbb{1}_2 & c\sigma \cdot \mathbf{p} \\ c\sigma \cdot \mathbf{p} & \left(\hat{V}_{\rm nuc} + \hat{v}_{\rm DCHF} - 2m_0c^2\right) \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} \psi_a^L(\vec{r}) \\ \psi_a^S(\vec{r}) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_a^L(\vec{r}) \\ \psi_a^S(\vec{r}) \end{pmatrix}, \quad \forall a$$

$$\varepsilon = E - m_0 c^2$$

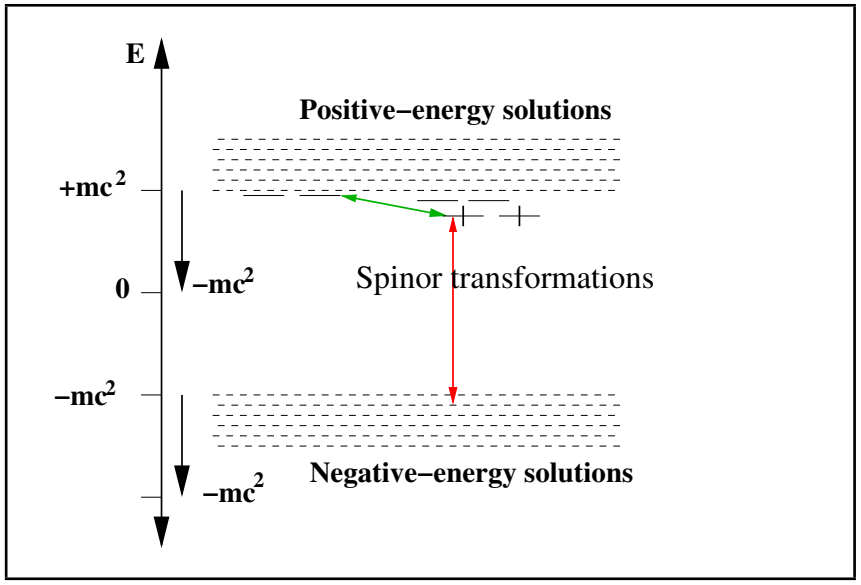
- Fock matrix for "frozen" atomic core

  1) Core energy: $\varepsilon_{\rm core} = \sum_{i,j>i}^{2N_{\rm core}} \left\{2\left\langle ij|ij\right\rangle - \left\langle ij|ji\right\rangle - \left\langle i\bar{j}|\bar{j}i\right\rangle\right\}$

  2) Inactive Fock matrix: $f_{pq}^{\rm DC} = h_{pq}^{\rm D} + \sum_{j}^{2N_{\rm core}} \left\{2\left\langle pj|qj\right\rangle - \left\langle pj|jq\right\rangle - \left\langle p\bar{j}|\bar{j}q\right\rangle\right\}$

1. Four-Component Electronic-Structure Theory

The "empty-Dirac" picture



- **Occupied** positive-energy bound-state spinors Fermi vacuum state $|0\rangle$
- **Empty** continuum of negative-energy states
- Expectation value of parameterized state vector
  $\left\langle Ref|\hat{H}|Ref\right\rangle = \left\langle 0|e^{-\hat{\kappa}}\hat{H}e^{\hat{\kappa}}|0\right\rangle$

- Approximation of general expectation value to first order:
  $\left\langle 0|e^{-\hat{\kappa}}\hat{H}^{DC}e^{\hat{\kappa}}|0\right\rangle \approx \left\langle 0|\left[\hat{H}^{DC},\hat{\kappa}\right]|0\right\rangle = \sum_{pq}\kappa_{pq}\left[\left\langle 0|\hat{H}^{DC}a_p^\dagger a_q|0\right\rangle - \left\langle 0|\hat{H}^{DC}a_q^\dagger a_p|0\right\rangle^*\right]$
- Parameterized Dirac-spinor transformations:
  $\hat{\kappa} = \sum_{pq}\left[\kappa_{p+q+}a_{p+}^\dagger a_{q+} + \kappa_{p+q-}a_{p+}^\dagger a_{q-} + \kappa_{p-q+}a_{p-}^\dagger a_{q+} + \kappa_{p-q-}a_{p-}^\dagger a_{q-}\right]$
- Green terms: minimization of energy w.r.t. rotations
- Red terms: maximization of energy w.r.t. rotations
  $\Rightarrow$ **minimax** variation

Four-Component Correlation Methods

. . . and why they are not more expensive than two-component ones

Integrals over positive-energy 4-spinors:

$$
\begin{aligned}
h^{+}_{mn} &= \left\langle \psi^{+}_{m} | \hat{h} | \psi^{+}_{n} \right\rangle = \left\langle \begin{pmatrix} \psi^{L}_{m} & \psi^{S}_{m} \end{pmatrix} | \begin{pmatrix} \hat{h}_{11} & \hat{h}_{12} \\ \hat{h}_{21} & \hat{h}_{22} \end{pmatrix} | \begin{pmatrix} \psi^{L}_{n} \\ \psi^{S}_{n} \end{pmatrix} \right\rangle \\
&= \left\langle \psi^{L}_{m} | \hat{h}_{11} | \psi^{L}_{n} \right\rangle + \left\langle \psi^{L}_{m} | \hat{h}_{12} | \psi^{S}_{n} \right\rangle + \left\langle \psi^{S}_{m} | \hat{h}_{21} | \psi^{L}_{n} \right\rangle + \left\langle \psi^{S}_{m} | \hat{h}_{22} | \psi^{S}_{n} \right\rangle \\
&= \sum_{J=1}^{N^L} \sum_{K=1}^{N^L} c^{L^*}_{mJ} \left\langle \phi^{L}_{J} | \hat{h}_{11} | \phi^{L}_{K} \right\rangle c^{L}_{nK} + \sum_{J=1}^{N^L} \sum_{K=1}^{N^S} c^{L^*}_{mJ} \left\langle \phi^{L}_{J} | \hat{h}_{12} | \phi^{S}_{K} \right\rangle c^{S}_{nK} \\
&+ \sum_{J=1}^{N^S} \sum_{K=1}^{N^L} c^{S^*}_{mJ} \left\langle \phi^{S}_{J} | \hat{h}_{21} | \phi^{L}_{K} \right\rangle c^{L}_{nK} + \sum_{J=1}^{N^S} \sum_{K=1}^{N^S} c^{S^*}_{mJ} \left\langle \phi^{S}_{J} | \hat{h}_{22} | \phi^{S}_{K} \right\rangle c^{S}_{nK}
\end{aligned}
$$

- Key: Four-component no-virtual-pair (NVP) approximation
- $dim[\mathcal{F}^{4c}] = dim[\mathcal{F}^{2c}]$
- Direct comparison of 4- and 2-component Hamiltonians possible

Special Relativity and Electron Correlation

Principal Approaches for Molecules

Spinor–based models

Hartree–Fock		*Dynamic Correlation*
2– or 4–component Hamiltonian	+	2– or 4–component Hamiltonian

Double–group MPPT/CI/CC

Spinorbital–based models

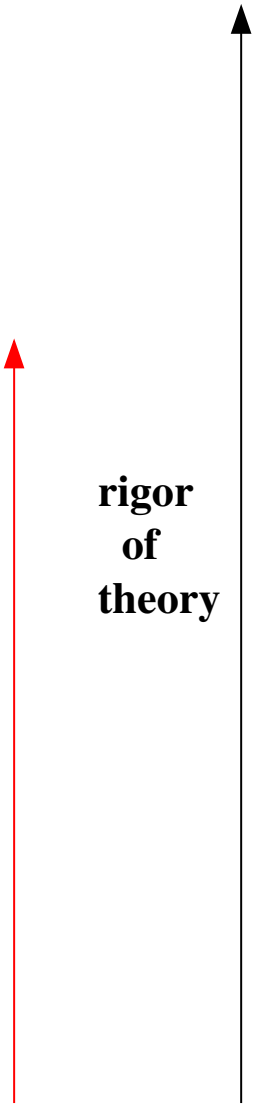
Hartree–Fock		*Dynamic Correlation*
scalar relativistic Hamiltonian	+	2–component Hamiltonian

Spin–orbit CI
Spin–orbit Coupled Cluster

Additive models

Hartree–Fock		*Dynamic Correlation*		*Magnetic Couplings*
scalar relativistic Hamiltonian	+	scalar relativistic Hamiltonian	+	2–component Hamiltonian

Spin–orbit QDPT
CASPT2–Spin–orbit RASSI



Spinors and Strings

General principles of rigorous relativistic correlation methods

General concept: Kramers-paired spinors

Time-reversal operator for a fermion:

$\hat{K} = e^{-\frac{\imath}{\hbar}\pi\left(\hat{\vec{s}}\cdot\vec{e}_y\right)}\,\hat{K}_0 = -\imath\Sigma_y\hat{K}_0$

Double group symmetry and quaternion algebra

Spinorbitals	General spinors
$\hat{K}\varphi_i\,\alpha = \varphi_i^*\,\beta$	$\hat{K}\phi_i = \phi_{\bar{i}}$
$\hat{K}\varphi_i^*\,\beta = -\varphi_i\,\alpha$	$\hat{K}\phi_{\bar{i}} = -\phi_i$

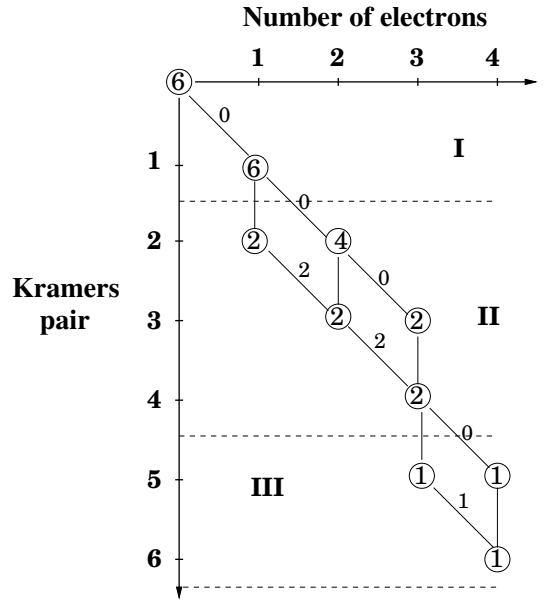
Spinor basis:

$\phi_i = a_i^\dagger \mid\rangle \qquad \phi_{\bar{i}} = a_{\bar{i}}^\dagger \mid\rangle$

- Many-particle wavefunction defined as
  - 1 unbarred (Kramers up) string $\mathcal{S} = a_i^\dagger a_j^\dagger a_k^\dagger \ldots$
  - 1 barred (Kramers down) string $\overline{\mathcal{S}} = a_{\bar{l}}^\dagger a_{\bar{m}}^\dagger a_{\bar{n}}^\dagger \ldots$

- Configuration Interaction: **Slater determinants**

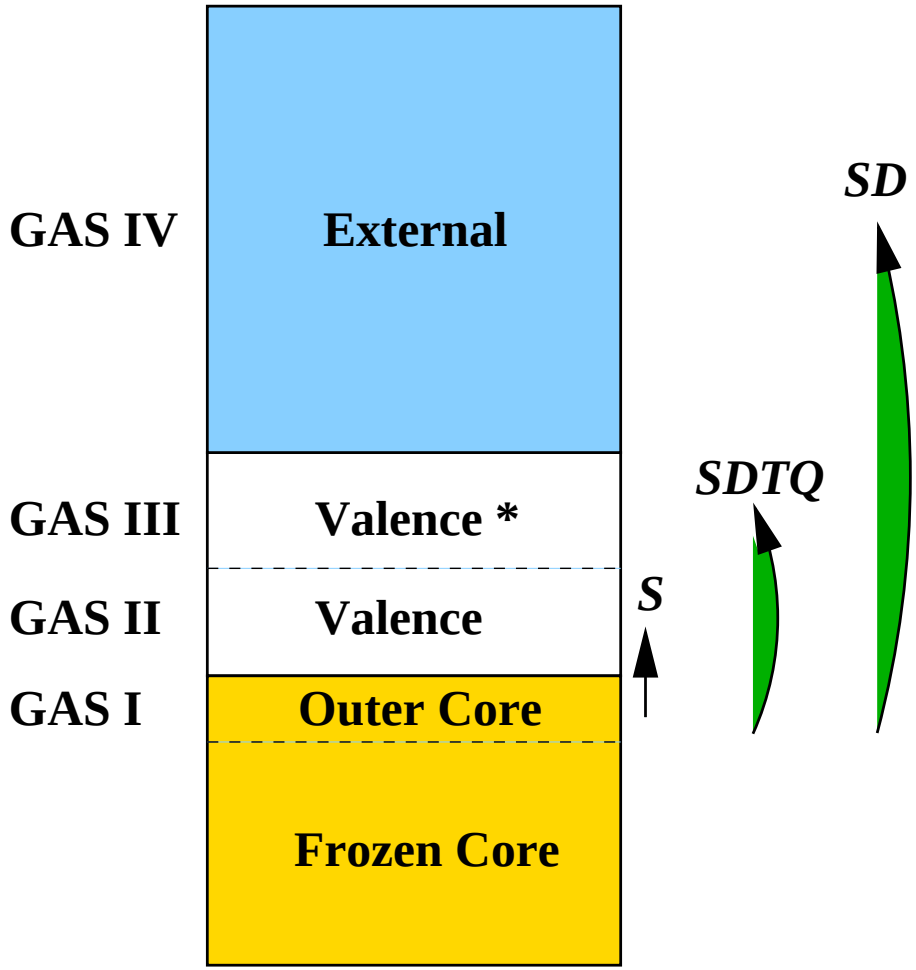
  Coupled Cluster: **Individual strings**



⊗ x: vertex weight
y: arc weight

Parameterization of the Wavefunction

Generalized Active Spaces



Special Relativity and Electron Correlation

Methods in comparison

Chalcogen homonuclear and heteronuclear diatomics[1]

Vertical excitation energies among π^{*2} state manifold

ΛS *States* $^3\Sigma^-, {}^1\Delta, {}^1\Sigma^+ \longrightarrow 0^+, 1, 2, 0^+, (\Omega)$

Splitting of $0^+, 1$ is a second-order spin-orbit effect

Purely molecular spin-orbit splitting

Contenders:

"Additive"[2]: *SO-DDCI3*, *SO-CASPT2*

"Non-additive"[3]: *4c-IH-FSCC*, *4c-GASCI*

[1] J.-B. Rota, S. Knecht, T. Fleig, D. Ganyushin, T. Saue, F. Neese, H. Bolvin *J Chem Phys* **135** (2011) *114106*

[2] F. Neese, *J Chem Phys* **119** (2003) *9428*

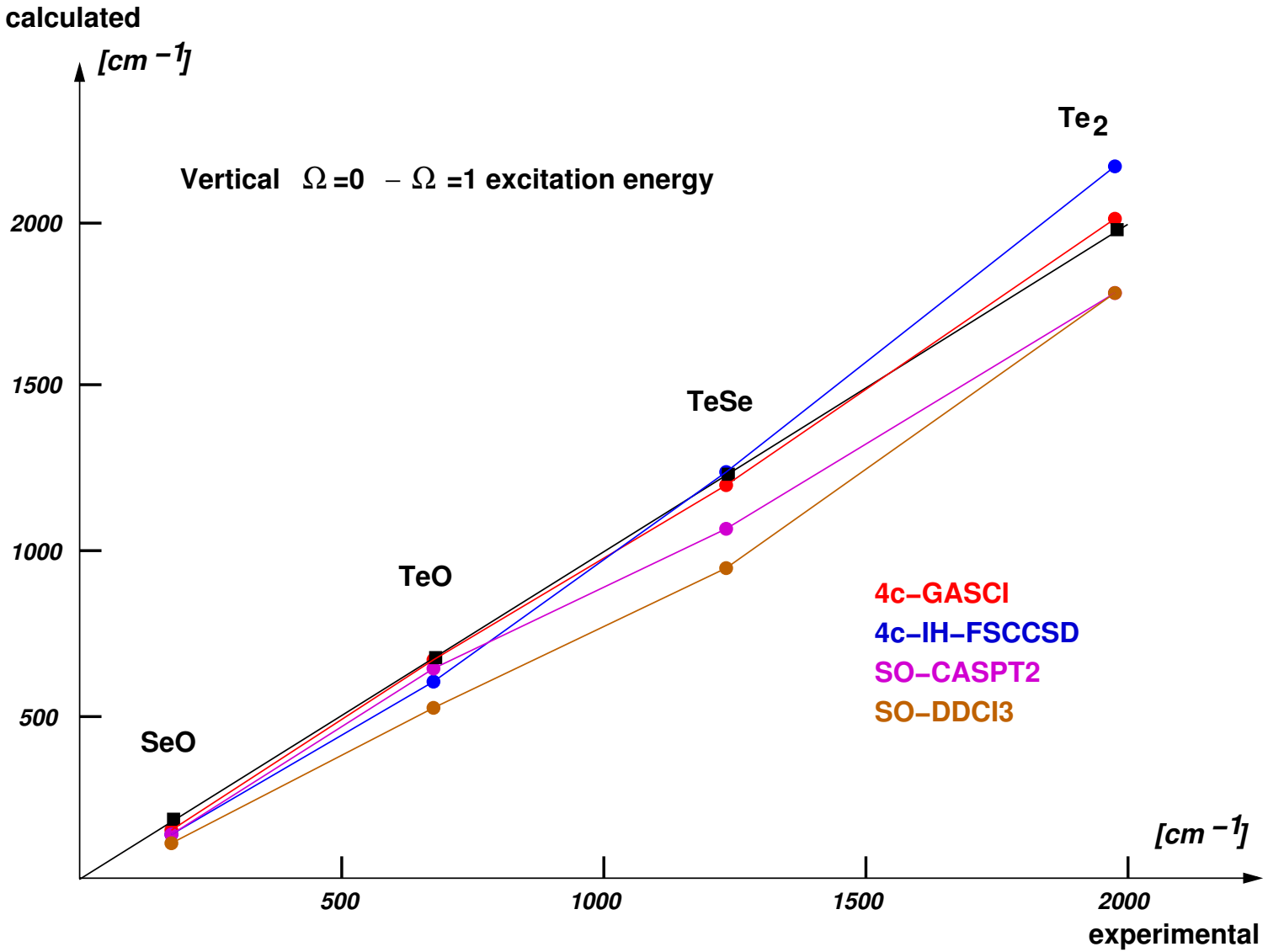
P.-Aa. Malmqvist, B.O. Roos, B. Schimmelpfennig, *Chem Phys Lett* **357** (2002) *357*

[3] L. Visscher, E. Eliav, U. Kaldor, *J Chem Phys* **115** (2001) *9720*

S. Knecht, H.J.Aa. Jensen, T. Fleig, *J Chem Phys* **132** (2010) *014108*

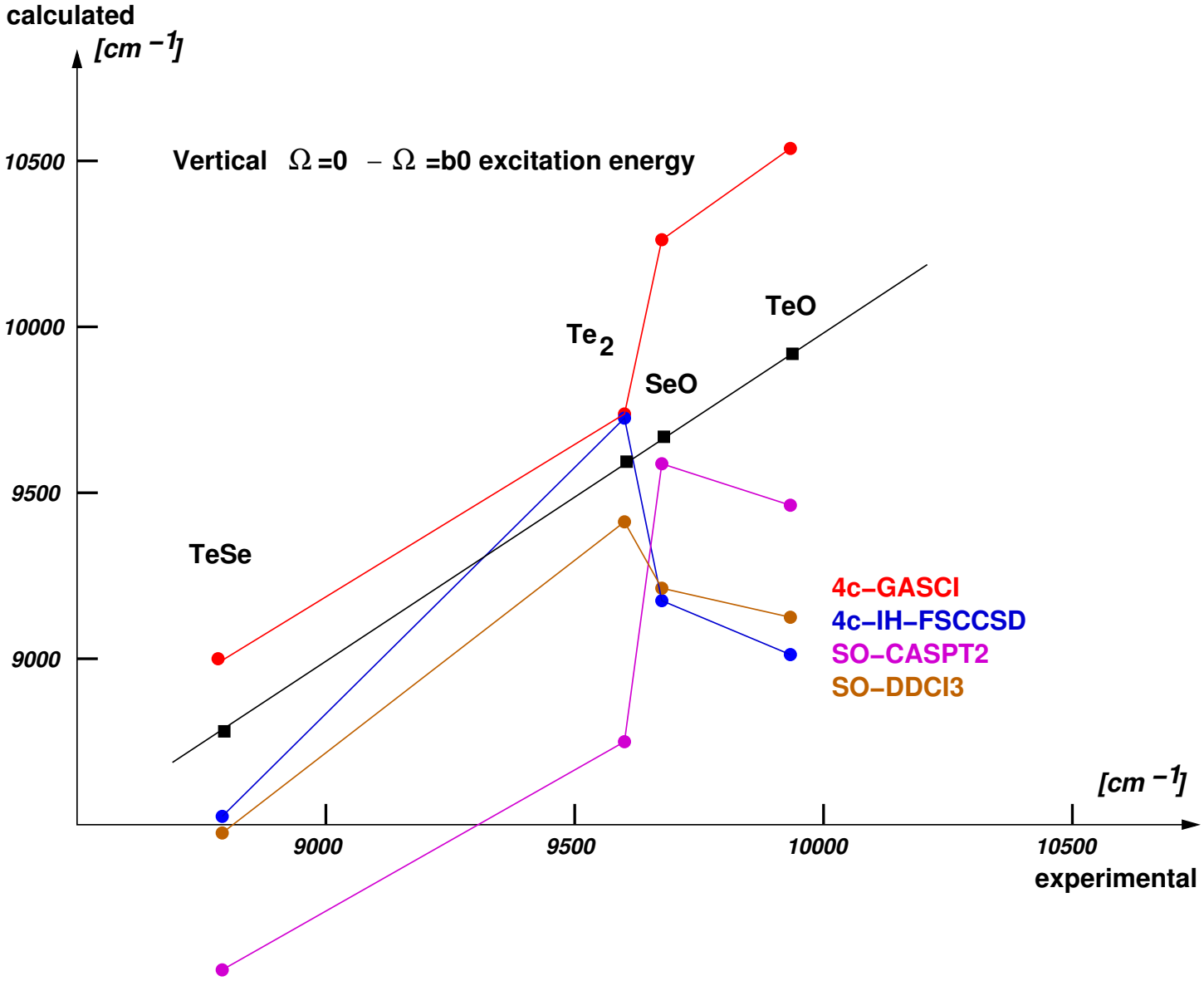
Special Relativity and Electron Correlation

Additive and non-additive methods in comparison



Special Relativity and Electron Correlation

Additive and non-additive methods in comparison



Special Relativity and Electron Correlation

Methods in comparison

Conclusions in the light of evidence

Non-additive, spinor-based methods largely superior for excitation energies

4c-GASCI allows for balanced treatment of ground and excited states

CI not size extensive

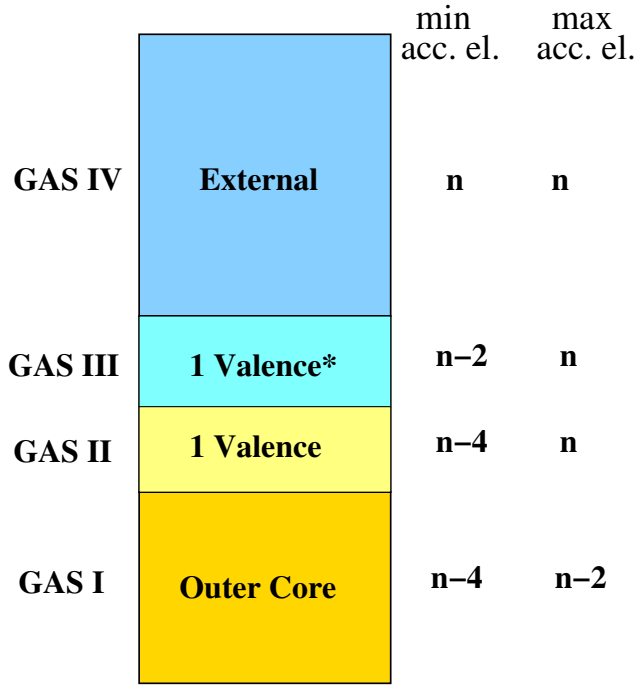
CI inefficient in treating higher excitations

Goal: More efficient spinor-based size-extensive electron correlation methods

Relativistic Generalized-Active-Space CC

L. K. Sørensen, J. Olsen, T. Fleig, *J Chem Phys* **134** (2011) *214102*
T. Fleig, L. K. Sørensen, J. Olsen, *Theo Chem Acc* **118,2** (2007) *347*
J. Olsen, *J Chem Phys* **113** (2000) *7140*

- "State-Selective" (SS) GAS-CC
  Generalized "Oliphant/Adamowicz" Ansatz[4]
- GAS-extended excitation manifold
  $\langle \mu_{\mathrm{GASCC}}| = \langle \psi^{\mathrm{Ref}}| \hat{\tau}^{\dagger}_{\mu_{\mathrm{GAS}}}$
- $\hat{\tau}_{\mu_{\mathrm{GAS}}}$ contains GAS-selected higher excitations
  $|\psi^{\mathrm{GASCC}}\rangle = exp(\sum_{\mu} t_{\mu}\hat{\tau}_{\mu_{\mathrm{GAS}}})\ |\psi^{\mathrm{Ref}}\rangle$
- Relativistic generalization of cluster operators
  $\hat{T}_1 = \sum_{ia} \left\{ t^a_i\hat{\tau}^a_i + t^{\bar{a}}_{\bar{i}}\hat{\tau}^{\bar{a}}_{\bar{i}} + t^{\bar{a}}_i\hat{\tau}^{\bar{a}}_i + t^a_{\bar{i}}\hat{\tau}^a_{\bar{i}} \right\}$; $\hat{T}_2 = \ldots$



Example for constructed higher excitations:

$$\langle \mu_{\mathrm{GASCC}}| = \left\langle \mu^{S(\mathrm{III}^1)}\right| + \left\langle \mu^{S(\mathrm{IV}^1)}\right| + \left\langle \mu^{D(\mathrm{III}^2)}\right| + \left\langle \mu^{D(\mathrm{IV}^2)}\right| + \left\langle \mu^{D(\mathrm{III}^1+\mathrm{IV}^1)}\right|$$
$$+\left\langle \boldsymbol{\mu}^{\mathbf{T}(\mathbf{III}^1+\mathbf{IV}^2)}\right| + \left\langle \boldsymbol{\mu}^{\mathbf{T}(\mathbf{III}^2+\mathbf{IV}^1)}\right| + \left\langle \boldsymbol{\mu}^{\mathbf{Q}(\mathbf{III}^2+\mathbf{IV}^2)}\right|$$

[4] N. Oliphant, L. Adamowicz *J Chem Phys* **94** (1991) *1229*

Relativistic Generalized-Active-Space CC

Electronic Ground States [5]

CC vector function

$$\Omega_\mu = \left\langle \mu \left| \left(\hat{H} + \left[\hat{H}, \hat{T} \right] + \tfrac{1}{2} \left[\left[\hat{H}, \hat{T} \right], \hat{T} \right] \tfrac{1}{6} \left[\left[\left[\hat{H}, \hat{T} \right], \hat{T} \right], \hat{T} \right] \ldots \right) \right| \mathrm{Ref} \right\rangle$$

- Loop over relativistic $N\Delta M_K$ classes of $\hat{H}, \hat{T}$
  Determines min./max. commutator nesting
  - Loop over commutator type, e.g. $\left[\left[\left[\hat{H}, \hat{T} \right], \hat{T} \right], \hat{T} \right]$
    - Loop over relativistic $N\Delta M_K$ classes of $\hat{T}$ operators
      Find all possible contractions
      - Loop over contractions and perform, e.g.

$$[[\hat{H}_{2v,2v}, \hat{T}_{2v,2o}], \hat{T}_{2v,2o}]$$
$$= \frac{1}{4} \sum_{abcd,i'j'a'b',i"j"a"b"} (ad|bc) t^{a'b'}_{i'j'} t^{a"b"}_{i"j"} a^\dagger_a a^\dagger_b \overbrace{a_c a_d a^\dagger_{a'} a^\dagger_{b'} a_{i'} a_{j'} a^\dagger_{a"}}^{} a^\dagger_{b"} a_{i"} a_{j"} .$$

[5] L. K. Sørensen, J. Olsen, T. Fleig, *J Chem Phys* **134** (2011) *214102*
L. K. Sørensen, T. Fleig, J. Olsen, *Z Phys Chem* **224** (2010) *999*

Relativistic Generalized-Active-Space CC[6]

Excitation Energies[7]

$$J^{CC}_{\mu} = \sum_{\nu} \left\langle \mu_{\mathrm{GAS}} | e^{-\hat{T}_{\mathrm{GAS}}} \left[\hat{H}, \hat{\tau}_{\nu_{\mathrm{GAS}}} \right] e^{\hat{T}_{\mathrm{GAS}}} | \psi^{\mathrm{Ref}} \right\rangle x_{\nu}$$

1. $|a\rangle = e^{\hat{T}_{\mathrm{GAS}}} \left|\psi^{\mathrm{Ref}}\right\rangle = \left(\sum_{k=0}^{\infty} \frac{1}{k!} \hat{T}^{k}_{\mathrm{GAS}} \right) \left|\psi^{\mathrm{Ref}}\right\rangle$

   $\hat{T}_{\mathrm{GAS}} \left|\psi^{\mathrm{Ref}}\right\rangle$ corresponds to calculating a sigma vector with amplitudes.

2. $|b\rangle = \left[\hat{H}, \hat{\tau}_{\nu_{\mathrm{GAS}}} \right] |a\rangle = \left(\hat{H}\hat{\tau}_{\nu_{\mathrm{GAS}}} - \hat{\tau}_{\nu_{\mathrm{GAS}}}\hat{H} \right) |a\rangle$ (CI sigma vectors)

3. $|c\rangle = e^{-\hat{T}_{\mathrm{GAS}}} |b\rangle = \left(\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \hat{T}^{k}_{\mathrm{GAS}} \right) |b\rangle$

4. $\Omega_{\mu_{\mathrm{GAS}}} = \langle \mu_{\mathrm{GAS}} | c \rangle = \left\langle \psi^{\mathrm{Ref}} \left| \hat{\tau}^{\dagger}_{\mu_{\mathrm{GAS}}} \right| c \right\rangle$ (CI transition density matrices)

Computational scaling:

CI-based implementation $O^{n+2}V^{n+2}$

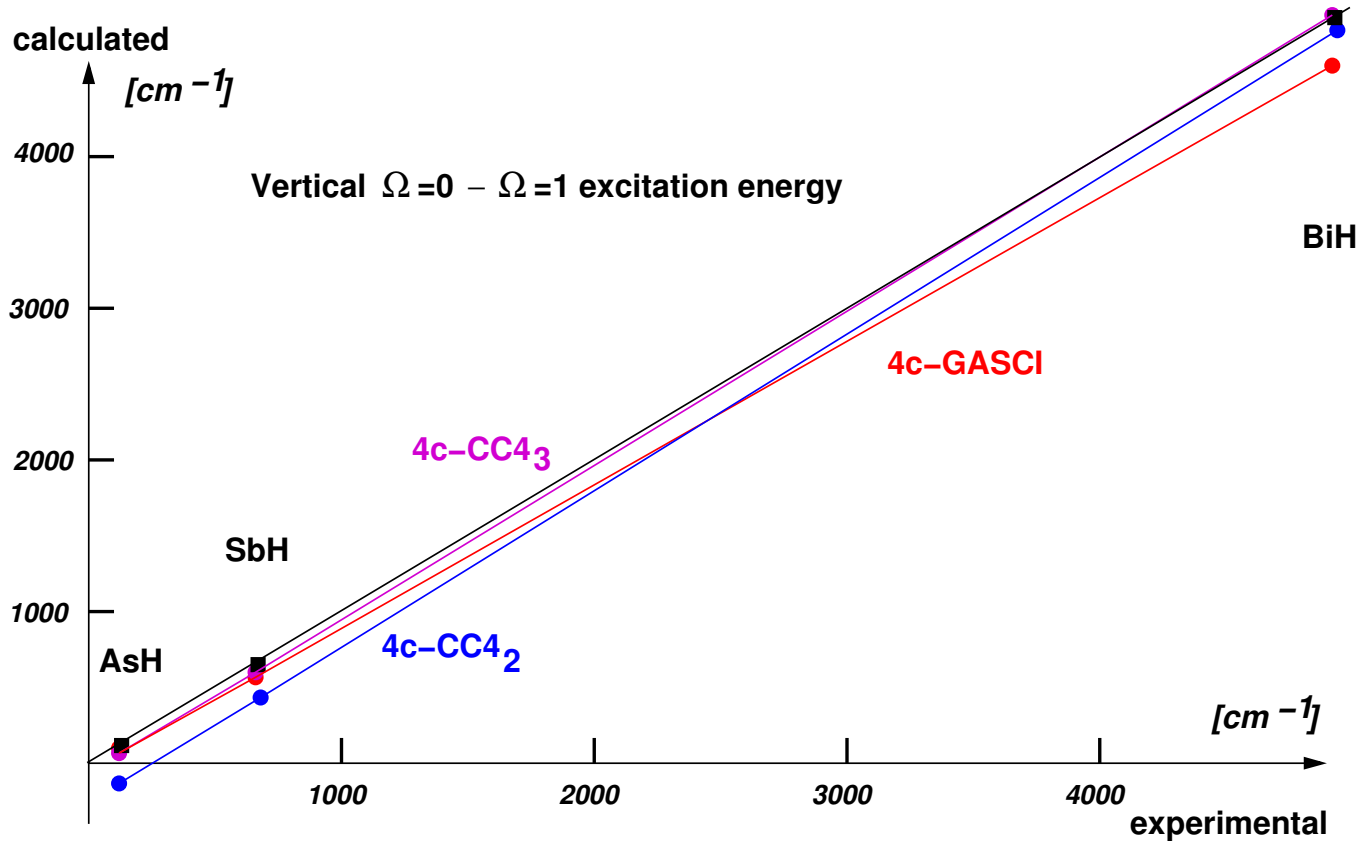
Conventional CC: $O^{n}V^{n+2}$

[6] M. Hubert, L. K. Sørensen, J. Olsen, T. Fleig, *Phys Rev A* **86** (2012) *012503*

[7] K. Hald, P. Jørgensen, J. Olsen, and M. Jaszuński, *J Chem Phys* **115** (2001) *671*

Series AsH, SbH, BiH

When is CC superior to GAS-CI?



- $CC4_3$ calculations consistently better than CAS-CISD[8]

[8] M. Hubert, L. K. Sørensen, J. Olsen, T. Fleig, *Phys Rev A* **86** (2012) *012503*

2. Correlated Wavefunction Theory for E_{eff}

The pseudo-scalar $\mathcal{PT}$-odd eEDM Hamiltonian:

- Salpeter's[9] modified Dirac equation:

$$\left[\gamma^{\mu}\left(-\imath\hbar\partial_{\mu}-\tfrac{e}{c}A_{\mu}\right)+m_0c\mathbb{1}_4\right]\psi(x)=\tfrac{d_e}{4}\,\gamma^0\gamma^5\,\left(\gamma^{\mu}\gamma^{\nu}-\gamma^{\nu}\gamma^{\mu}\right)F_{\mu\nu}\,\psi(x)$$

- from which the eEDM operator can we written as an expectation value:

$$\left\langle -d_e\gamma^0\boldsymbol{\Sigma}\cdot\mathbf{E}\right\rangle_{\psi_H}=\tfrac{2\imath cd_e}{e\hbar}\left\langle\gamma^0\gamma^5\vec{p}^{\,2}\right\rangle_{\psi_H}$$

- Requires kinetic-energy integrals of the type:

$$\left\langle\psi^L|\vec{p}^{\,2}|\psi^S\right\rangle$$

- and therefore explicitly the Small-component wave functions.
- Implemented in the `DIRAC11` program package[10]

[9] E. Salpeter, *Phys Rev* **112** (1958) *1642*

[10] DIRAC, a relativistic ab initio electronic structure program, Release DIRAC11 (2011), written by R. Bast, H. J. Aa. Jensen, T. Saue, L. Visscher, et al.

2. Correlated Wavefunction Theory for E_{eff}

Configuration Interaction Expectation Value

- Dirac-Coulomb Hamiltonian operator

$$\hat{H}^{DC} = \sum_A \sum_i \left[c(\vec{\alpha} \cdot \vec{p})_i + \beta_i m_0 c^2 + V_{iA} \right] + \sum_{i,j>i} \frac{1}{r_{ij}} \mathbb{1}_4 + \sum_{A,B>A} V_{AB}$$

- All-electron Dirac-Coulomb Hartree-Fock (DCHF) calculation

  set of time-reversal paired 4-spinors $\hat{K}\varphi_i = \varphi_{\bar{i}}$ and $\hat{K}\varphi_{\bar{i}} = -\varphi_i$

- Expansion and variation in N-electron sector of Fock space

$$|\psi_k\rangle = \sum_{I=1}^{\dim \mathcal{F}^{\mathrm{t}}(\mathrm{M,N})} c_{kI} \left| (\mathcal{S}\overline{\mathcal{T}})_I \right\rangle$$

- Expectation value with eEDM interaction Hamiltonian[11]

$$\left\langle \hat{H}_{\mathrm{edm}} \right\rangle_{\psi_k} = \sum_{I,J=1}^{\dim \mathcal{F}^{\mathrm{t}}(\mathrm{M,N})} c^*_{kI} c_{kJ} \left\langle (\mathcal{S}\overline{\mathcal{T}})_I \right| \sum_{i=1}^{N} \hat{H}_{\mathrm{edm}}(i) \left| (\mathcal{S}\overline{\mathcal{T}})_J \right\rangle$$

[11] T. Fleig and M. K. Nayak, submitted.

3. HfF^+ Electronic Structure and EDM Interaction Constant

GAS-CI definitions

- Basis: uncontracted vTZ
  Hf: $\{30s, 24p, 15d, 10f, 3g, 1h\}$
  F: $\{10s, 5p, 2d, 1f\}$
- Dirac-Coulomb Hamiltonian
- Full $(SS|**)$ integrals (EDM)

	# of Kramers pairs	accumulated # of electrons min.	max.
Virtual Kramers pairs	118	34	34
Hf: 6s, 5d	6	34–p	34
F: 2s, 2p	4	32–(m+n)	32
Hf: 5s, 5p F: 1s	5	24–m	24
Hf: 4f	7	14–q	14
Frozen core	(23)		

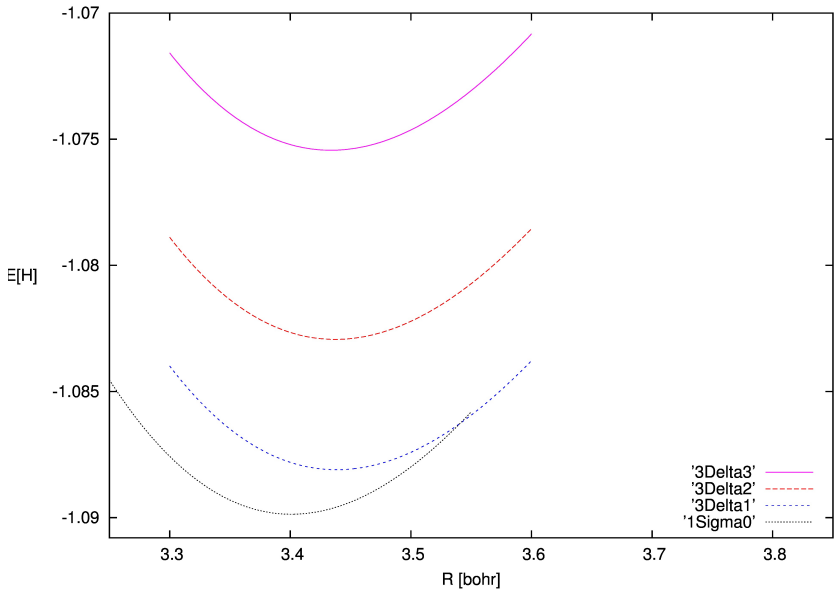
HfF^+ electronic states and spectroscopic constants

$\Omega = 3$ $(Hf^{2+}6s^15d^1)$

$\Omega = 2$ $(Hf^{2+}6s^15d^1)$

$\Omega = 1$ $(Hf^{2+}6s^15d^1)$

$\Omega = 0$ $(Hf^{2+}6s^2)$



	R_e [a.u.]				ω_e [cm^{-1}]			
Model	$\Omega = 0$	$\Omega = 1$	$\Omega = 2$	$\Omega = 3$	$\Omega = 0$	$\Omega = 1$	$\Omega = 2$	$\Omega = 3$
CAS-CI(10)	3.400	3.436	3.434	3.431	796	774	775	778
MR-CISD(10)	3.506	3.558	3.557	3.552	656	643	643	644
MR-CISD+T(10)	3.510	3.560			654	643		
MR-CISD(20)	3.401	3.438	3.437	3.434	800	768	769	772
Experiment[12]					790.76	760.9		
Experiment[13]	3.374	3.407			791.2	761.3	762.3	761.5

[l] K. Cossel et al., *Chem. Phys. Lett.* **546** (2012) *1*

[m] B.B. Barker, I.O. Antonov, V.E. Bondybey, M.C. Heaven, *J Chem Phys* **134** (2011) *201102*

HfF^+ spectroscopy; excitation energies

Model	T_e [cm^{-1}] $\Omega=0$	$\Omega=1$	$\Omega=2$	$\Omega=3$	$T_v^{3.4[a.u.]}$ [cm^{-1}] $\Omega=0$	$\Omega=1$
CAS-CI(10)	1543	0	1058	2480	1488	0
MR-CISD(10)	65	0	1007	2487	0	358
MR-CISD+T(10)	0	25			0	442
MR-CISD(20)	0	387	1521	3166	0	451
MR-CISD+T(20)					0	679
Experiment[14]	0	993	2166	3951		

- Active-space triples correction gives important contribution.
- Estimated MR-CISD+T(20) value for $T_e \approx 1180\ cm^{-1} (\Omega = 1)$
- Ongoing investigation of full PECs, transition dipole moments, and vibrational states

[14] B.B. Barker, I.O. Antonov, V.E. Bondybey, M.C. Heaven, *J Chem Phys* **134** (2011) *201102*

HfF^+: E_{eff} in the $\Omega = 1$ science state[15]

Model	$E_{\mathrm{eff}}\ \left[\frac{\mathrm{GV}}{\mathrm{cm}}\right]$
CAS-CI(10)	24.1
MR-CISD(10)	22.4
MR-CISD(20)	23.3
MR-CISD+T(20)	23.7
MR-CISD(34)	22.9
MR-CISD(34)+T	23.3
Estimate, Meyer et al.[16]	≈ 30
20 e^- corr., Titov et al.[17]	24.2

(+) All-electron calculation

(+) No configuration selection

(+) Spinors as one-particle basis functions

(+) Dirac-Coulomb Hamiltonian

(-) Basis-set incompleteness
→ vQZ corrections

(-) Higher excitations
→ CC expectation values

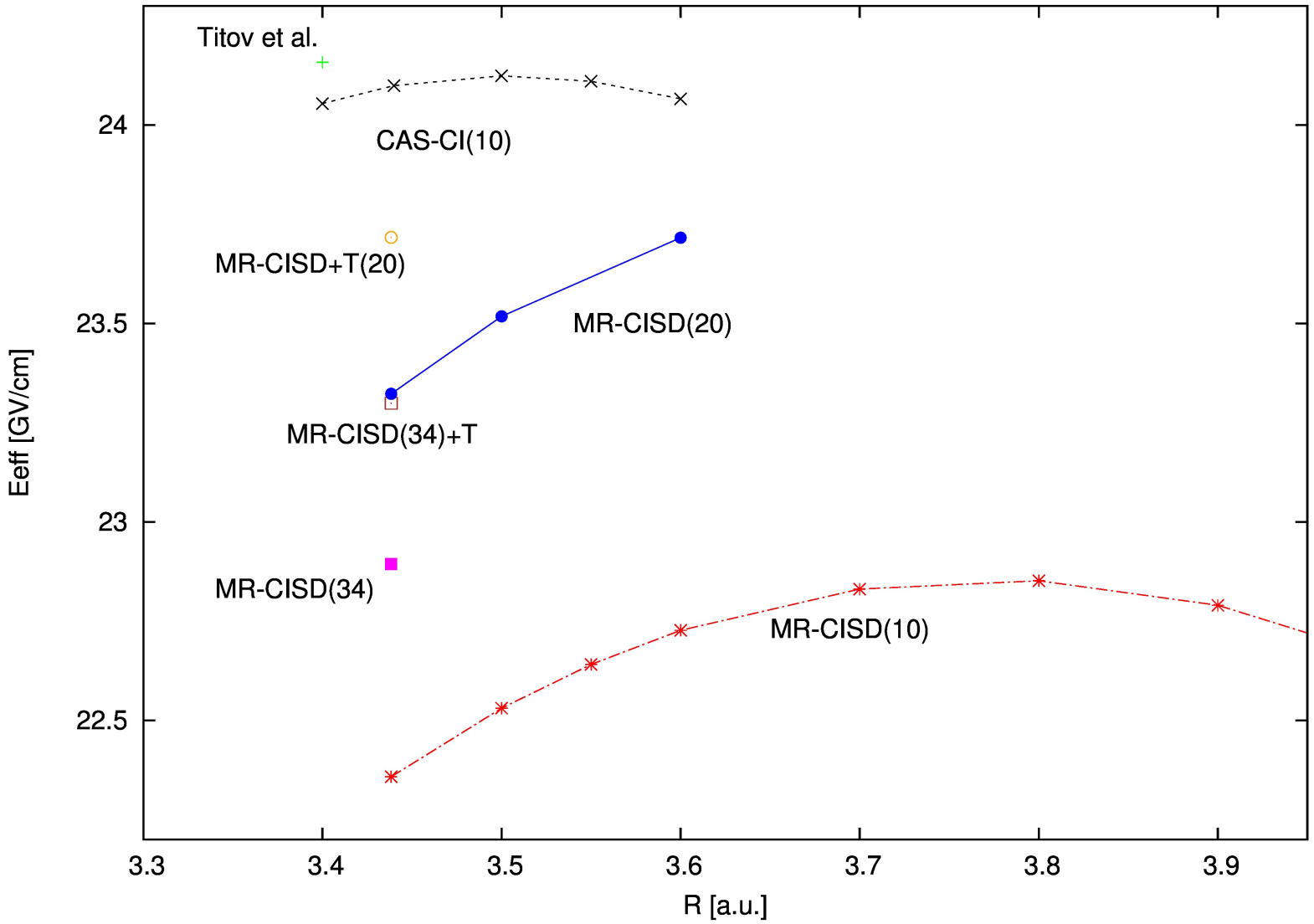
[15] T. Fleig and M. K. Nayak, submitted.

[16] A.N. Petrov, N.S. Mosyagin, T.A. Isaev, A.V. Titov, *Phys Rev A* **76** (2007) *030501(R)*

[17] E.R. Meyer, J.L. Bohn, *Phys Rev A* **78** (2008) *010502(R)*

The eEDM in a molecular framework

$\left\langle \hat{H}_{\rm edm} \right\rangle_{\psi_{\Omega=1}}$ as a function of R



Ongoing Work

- Commutator-based GER CC Jacobian, non-relativistic version
  (with Mickael Hubert and Jeppe Olsen)
- Commutator-based GER CC Jacobian, relativistic version
  (with Mickael Hubert and Lasse Sørensen)
- 4-component Gaunt / Breit operator in correlated approaches
  (with Jessica Loras)
- 4-Component commutator-based GER CC expectation values
  (with Avijit Shee and Malika Denis)

Future Work

Blanc proposal, submitted January 2013.

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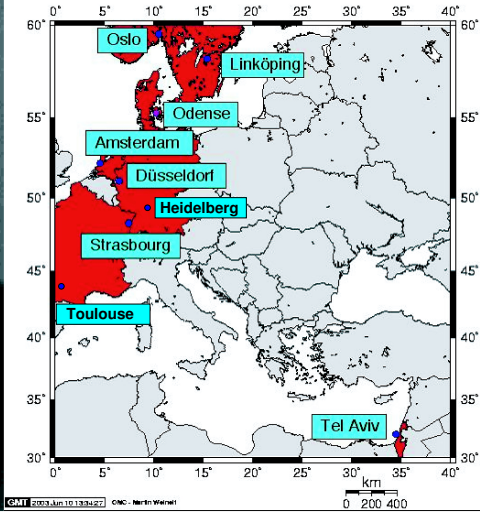
ThO, ThF^+, WC
other $\mathcal{P}$- and $\mathcal{P},\mathcal{T}$-nonconserving operators

DIRAC a metalaboratory for the development of relativistic 4- and 2-component electronic-structure methodology

P rogram
• for
A tomic
• and
M olecular

D irect
I terative
R elativistic
A ll-electron
C alculations



- `KR-CI`.
  `Kramers-Restricted GAS Configuration Interaction Program`
  (released in DIRAC10/DIRAC11/DIRAC12)
  Authors: S Knecht, T Fleig, J Olsen, HJAa Jensen

- `KR-CC`.
  `Kramers-Restricted GAS Coupled Cluster Program`
  (not yet released)
  Authors: LK Sørensen, J Olsen, M Hubert, T Fleig