New development of internally contracted MRCI

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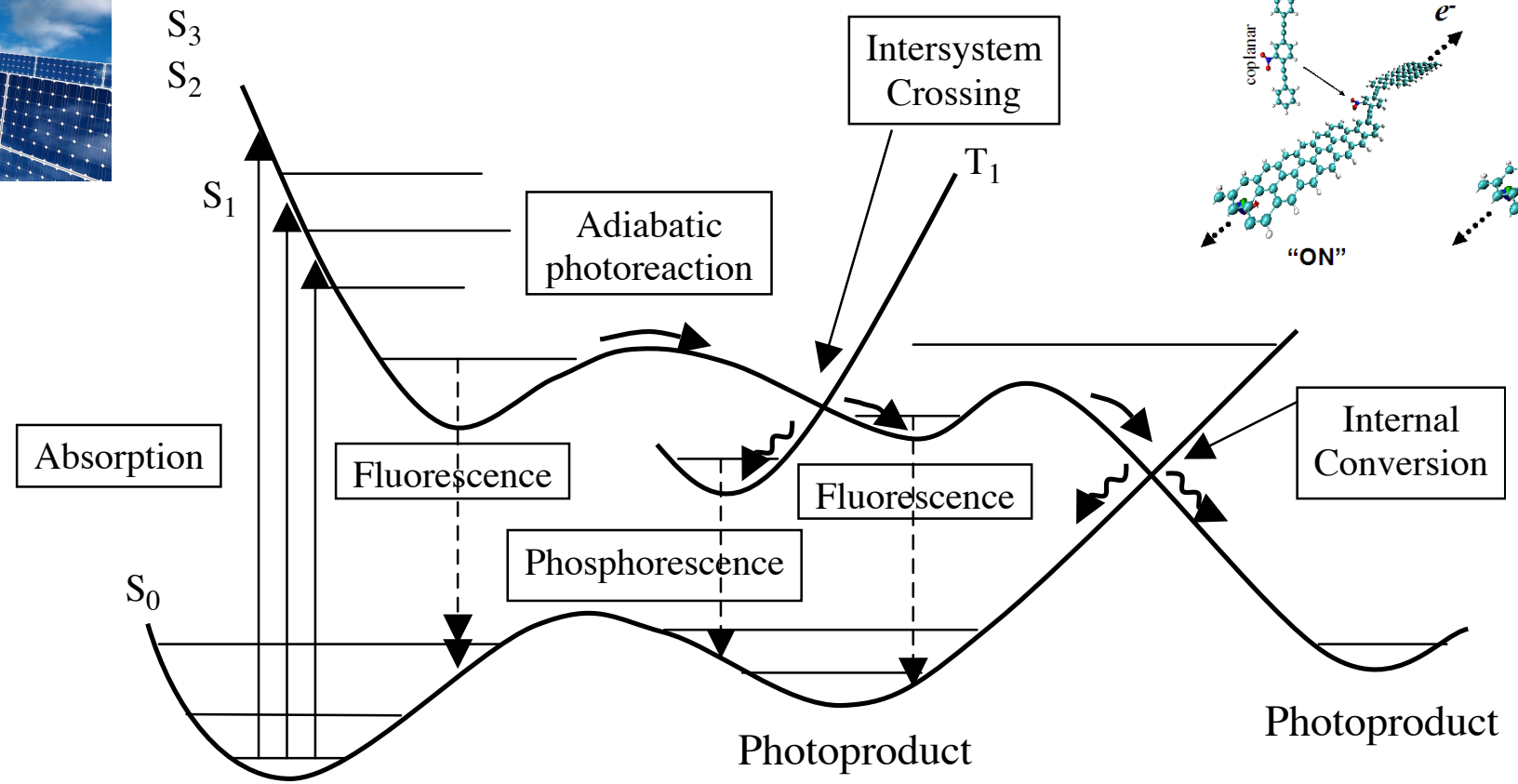
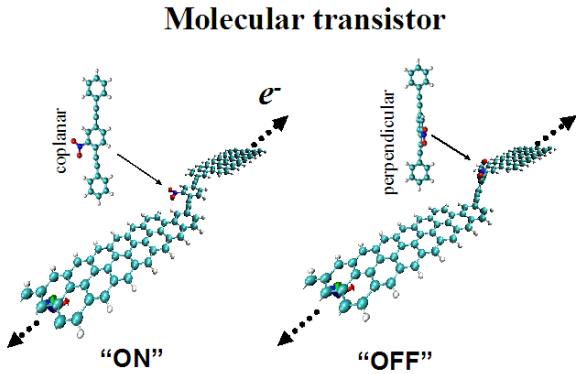
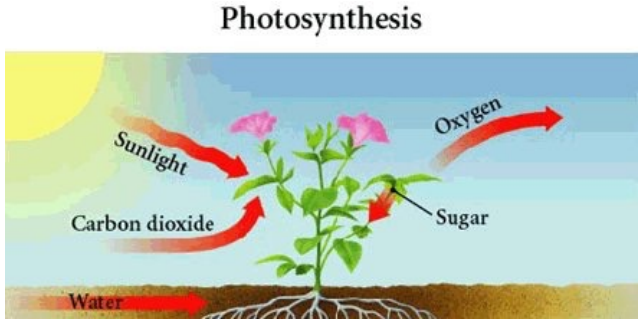
Contains

- ***Excited state and none-adiabatic problem***
- ***EN-GMFCI***
- icMRCI based on GUGA

Photo-physics and ***photo-chemistry*** procedures

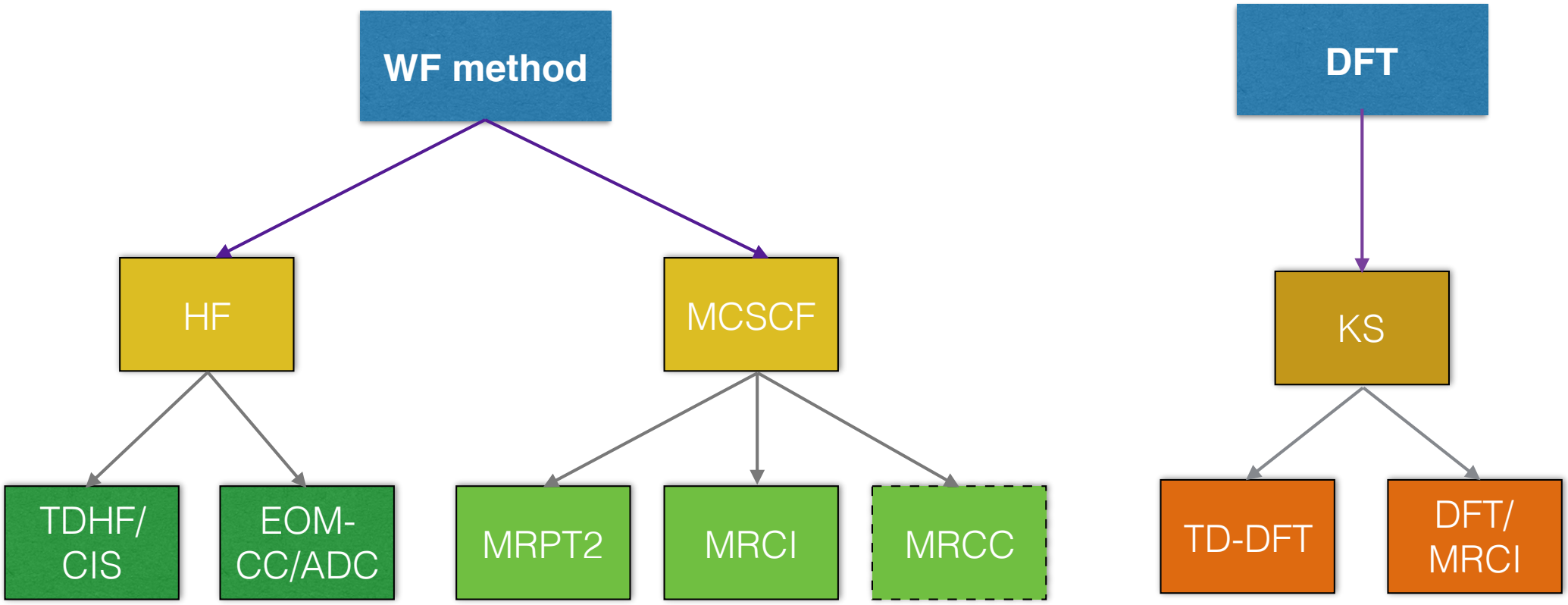






TheoChem, 729,99-108,2005

Methods for the excited state



Beijing ***D***ensity ***F***unctional ***p***ackage- ***BDF***

- SCF level

  RHF, UHF, ROHF, RKS, UKS,ROKS - Direct and none-direct, point group symmetry, CD/RI approximation.

  DFT functional: LDA,GGA,Hybrid, range-sep Hybrid etc.

- MCSCF.

- Post SCF and excited states

  MP2, Frag-LMP2

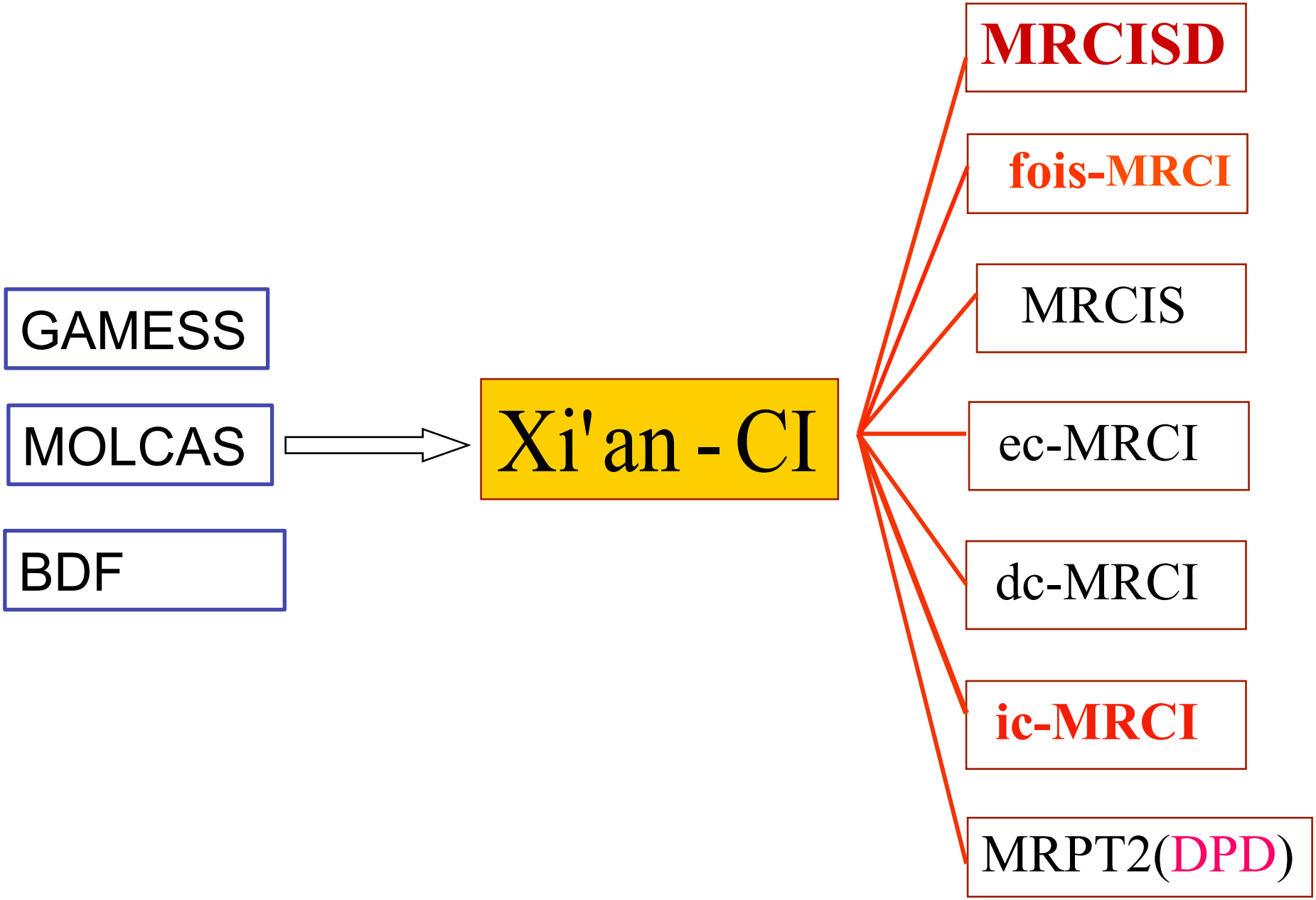
  TDDFT/TDHF, TDDFT+SOC, TD Gradient and NAC

  CCSD,CCSD(T), ***EOM-IP/EA/EE,CCSD+SOC***

  MRCI,MRPT2, MRCI-SOC,MCCEPA

  EN-GMFCI

Xi'an-CI package



Contains

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- ***EN-GMFCI***
- icMRCI based on GUGA

Electron-Nuclei General mean field configuration interaction

$$\hat{H}(\vec{R}^e, \vec{Q}) = \hat{H}(\vec{R}^e) + \hat{H}(\vec{Q}) + \hat{H}(\vec{R}^e, \vec{Q})$$

$$\hat{H}(\vec{R}^e) = -\frac{1}{2}\sum_{i=1}^{p} \nabla^2_{\vec{r}^e_i} + \sum_{1\le i<j\le p} \frac{1}{||\vec{r}^e_i - \vec{r}^e_j||}$$ Electron

$$\hat{H}(\vec{Q}) = -\frac{1}{2}\sum_{i=1}^{q} \nabla^2_{\vec{Q}_i} + \sum_{1\le a<b\le N} \frac{Z_a Z_b}{||\vec{r}^e_i - \vec{r}^0_a - \hat{G}_a^{-1}\hat{L}^T\vec{Q} - \hat{G}_b^{-1}\hat{L}^T\vec{Q}||}$$

Nuclei

$$\hat{H}(\vec{Q}, \vec{R}^e) = -\sum_{i}^{p}\sum_{a}^{N} \frac{Z_a Z_b}{||\vec{r}^e_i - \vec{r}^0_a - \hat{G}_a^{-1}\hat{L}^T\vec{Q}||}$$ Coupling term

P. Cassam-Chenai, B. Suo, W. Liu, Phys. Rev. A,92,012502,2015.

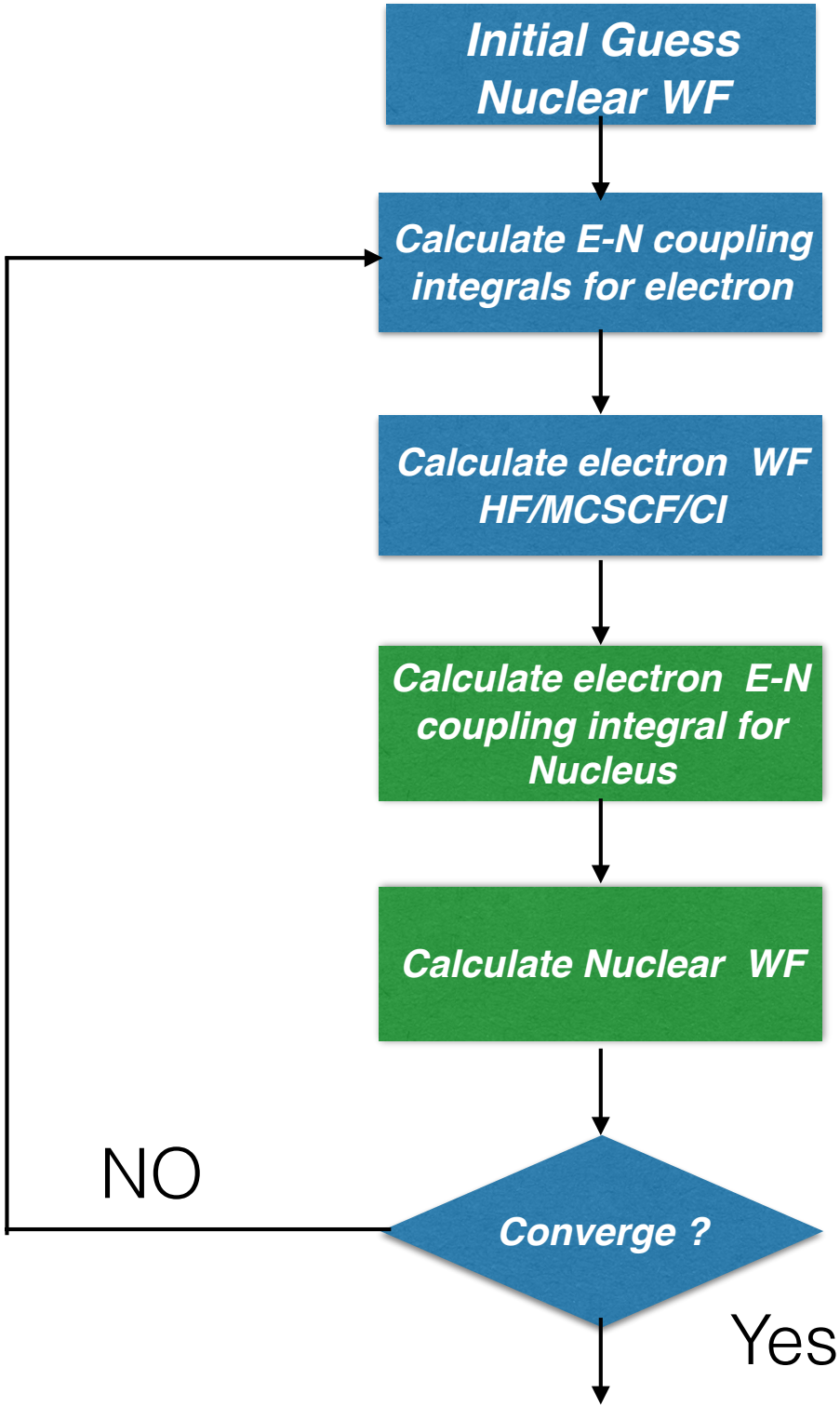
General Mean field approach

Electrons are in a mean field generated by nucleus

$$\hat{H}^{eff}(\vec{R}^e) = \hat{H}(\vec{R}^e) + \langle \phi_{\vec{0}}^{(0)}(\vec{Q}) | \hat{H}(\vec{Q}) + \hat{H}(\vec{R}^e, \vec{Q}) | \phi_{\vec{0}}^{(0)}(\vec{Q}) \rangle_{\vec{Q}}$$

Nucleus are in a mean field generated by electrons

$$\hat{H}^{eff}(\vec{Q}) = \hat{H}(\vec{Q}) + \langle \phi_{\vec{0}}^{(1)}(\vec{R}^e) | \hat{H}(\vec{R}^e) + \hat{H}(\vec{R}^e, \vec{Q}) | \phi_{\vec{0}}^{(1)}(\vec{R}^e) \rangle_{\vec{R}^e}$$

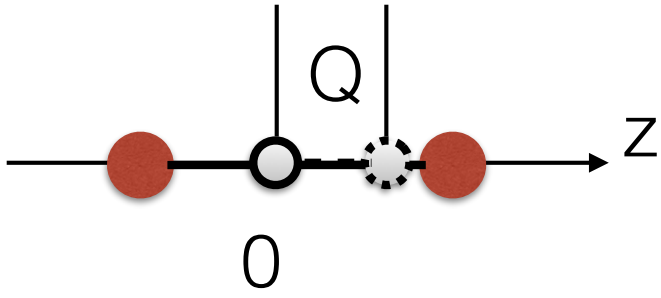


Self-consistent solving EN general mean field problem is solved.

Configuration interaction can be evoked based on mean field result.

$$|\Phi_{ni}(\vec{Q},\vec{R}\rangle = |\phi_n(\vec{Q})\rangle|\phi_i(\vec{R}^e)\rangle$$

For diatomic molecule



$$Q = \sqrt{\mu_{ab}}(r_{a_z} - r^0_{a_z} - r_b + r^0_{b_z}) \qquad \mu_{ab} = \frac{m_a m_b}{m_a + m_b}$$

Nucleus

$$\hat{H}^{eff}(Q) = -\frac{1}{2}\sum_{i=1}^{q}\nabla^2_{Q_i} + \frac{\sqrt{\mu_{ab}}Z_a Z_b}{|\xi^0_{ab} + Q|} + \langle\phi^{(1)}_{\vec{0}}(\vec{R^e})| - \frac{1}{2}\sum_{i=1}^{p}\nabla^2_{\vec{r^e_i}} + \sum_{1\le i<j\le p}\frac{1}{\|\vec{r}_i{}^e - \vec{r}_j{}^e\|}$$

$$-\sum_{i=1}^{p}\frac{Z_a}{\sqrt{(r^e_{i_x})^2 + (r^e_{i_y})^2 + (r^e_{i_z} - r^0_{a_z} - \frac{\sqrt{\mu_{ab}}Q}{m_a})^2}} + \frac{Z_b}{\sqrt{(r^e_{i_x})^2 + (r^e_{i_y})^2 + (r^e_{i_z} - r^0_{b_z} + \frac{\sqrt{\mu_{ab}}Q}{m_b})^2}}|\phi^{(1)}_{\vec{0}}(\vec{R^e})\rangle_{\vec{R^e}}$$

Electron

$$\hat{H}^{eff}(\vec{R^e}) = -\frac{1}{2}\sum_{i=1}^{p}\nabla^2_{\vec{r^e_i}} + \sum_{1\le i<j\le p}\frac{1}{\|\vec{r}_i{}^e - \vec{r}_j{}^e\|} + \langle\phi^{(0)}_0(Q)| - \frac{1}{2}\nabla^2_Q + \frac{\sqrt{\mu_{ab}}Z_a Z_b}{|\xi^0_{ab} + Q|}$$

$$-\sum_{i=1}^{p}\frac{Z_a}{\sqrt{(r^e_{i_x})^2 + (r^e_{i_y})^2 + (r^e_{i_z} - r^0_{a_z} - \frac{\sqrt{\mu_{ab}}Q}{m_a})^2}} + \frac{Z_b}{\sqrt{(r^e_{i_x})^2 + (r^e_{i_y})^2 + (r^e_{i_z} - r^0_{b_z} + \frac{\sqrt{\mu_{ab}}Q}{m_b})^2}}|\phi^{(0)}_0(Q)\rangle_Q$$

Nuclear wave function

Kratzer potential

$$[\frac{\hbar^2}{2\mu}(-\frac{\partial^2}{\partial r^2}+\frac{J(J+1)}{r^2})+\frac{A}{r^2}-\frac{B}{r}]\psi_n^j(r)=E_{nj}\psi_n^n(r)$$

Reduced formula from Kratzer $x=\frac{r}{r_e}$

$$\{-\frac{\partial^2}{\partial x^2}+K(\frac{1}{x^2}-\frac{2}{x})\}\psi_n^j(x)]=\epsilon_{nj}\psi_n^j(x)$$

$$K=J(J+1)+A\frac{2\mu}{\hbar^2}$$

D. Secrest,JCP,89,1017,1988

EN coupling integrals

$$I_{e-n}[Z_I, r^0_{I_z}, \eta] = \langle \phi^{kra}_i(Q)\chi_1(\vec{r^e})| \frac{Z_I}{\sqrt{(r^e_x)^2 + (r^e_y)^2 + (r^e_z - r^0_{I_z} + \eta Q)^2}} |\phi^{kra}_j(Q)\chi_2(\vec{r^e})\rangle$$

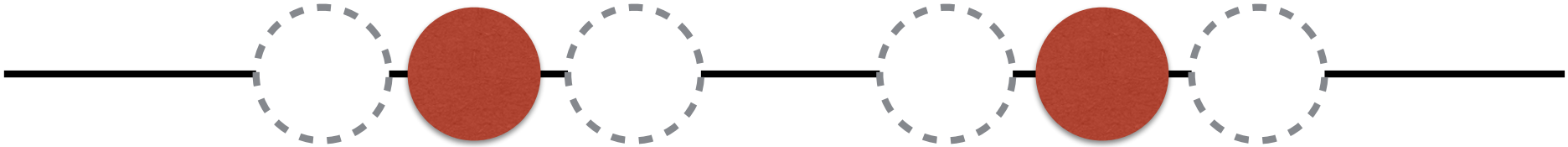
Here, the Kratzer functions are

$$\phi^{kra}_i(Q) = \frac{N^{kra}_i}{\sqrt{\xi^0_{ab}}} \left(1 + \frac{Q}{\xi^0_{ab}}\right)^{\lambda} Exp\left[\frac{\lambda(1-\lambda)}{\lambda + i}(1 + \frac{Q}{\xi^0_{ab}})\right] \; {}_1F_1[-i, 2\lambda; \frac{2\lambda(\lambda-1)}{\lambda+i}\left(1 + \frac{Q}{\xi^0_{ab}}\right)]$$

1 Rys and generalized Laguerre double quadrature formulas
2 Multi-Precision based on library arprec

P. Cassam-Chenia, B. Suo, W. Liu, Phys. Rev. A,92,012502,2015.

Off-center basis:



H_2, Convergence of total energy with number of Kratz and Off-center basis, Full-CI, cc-PVTZ

	K=4	K=8	K=12	K=16
n=4	-1.1621504	-1.1622377	-1.1622418	-1.1622419
n=8	-1.1623184	-1.1624301	-1.1624334	-1.1624341
n=12	-1.1623574	-1.1624676	-1.1624750	-1.1624754
n=16	-1.1623877	-1.1624996	-1.1625050	-1.1625060

Convergence of EN-GMFCI energy with basis sets and off-center basis

	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV5Z
n=4	-1.1576745 (18,0)	-1.1622419 (36,0)	-1.1632984 (68,0)	-1.1636441 (118,0)
n=8	-1.1579290 (26,5)	-1.1624380 (44,4)	-1.1634754 (76,2)	-1.1638262 (126,0)
n=12	-1.1581072 (34,10)	-1.1624953 (52,9)	-1.1636184 (84,5)	-1.1638365 (134,5)
n=16	-1.1581475 (42,16)	-1.1625060 (60,16)	-1.1635140 (92,10)	-1.1638438 (142,8)

Two numbers in parentheses are number of basis functions and number of basis functions should be eliminated due to basis set linear dependent.

Full CI v.s. Limited CI

	Full CI	Limited CI	
Numbers of CSF's	144720	6286	**4.4%**
E^0 (hartree)	-1.1638438	-1.1638413	
v; 0 —> 1 (cm^{-1})	4165.36	4165.86	

cc-pV5Z, n=16

Transition	TF-NOMO/CIS	TF-NOMO/FCI	This work	Exp.
		H_2		
v: 0 —>1	4655	4182	4165	4161
v: 0 —>2	9406	NA	8110	8087
Σ_g^+ : 0 —>1	106556	NA	91711	91700
		D_2		
v: 0 —>1	3549	3006	2994	2994
v: 0 —>2	7026	NA	5874	5869
Σ_g^+: 0 —>1	107628	NA	92182	91697
		T_2		
v: 0 —>1	2929	2477	2465	2465
v: 0 —>2	5843	NA	4851	4849
Σ_g^+ : 0 —>1	108043	NA	92375	91696

A brief summary

- Electron-Nuclei Mean field approximation
- EN-SCF/MCSCF/MRCI
- EN-FCI (direct product of electron and nucleus)
- Off-center basis sets

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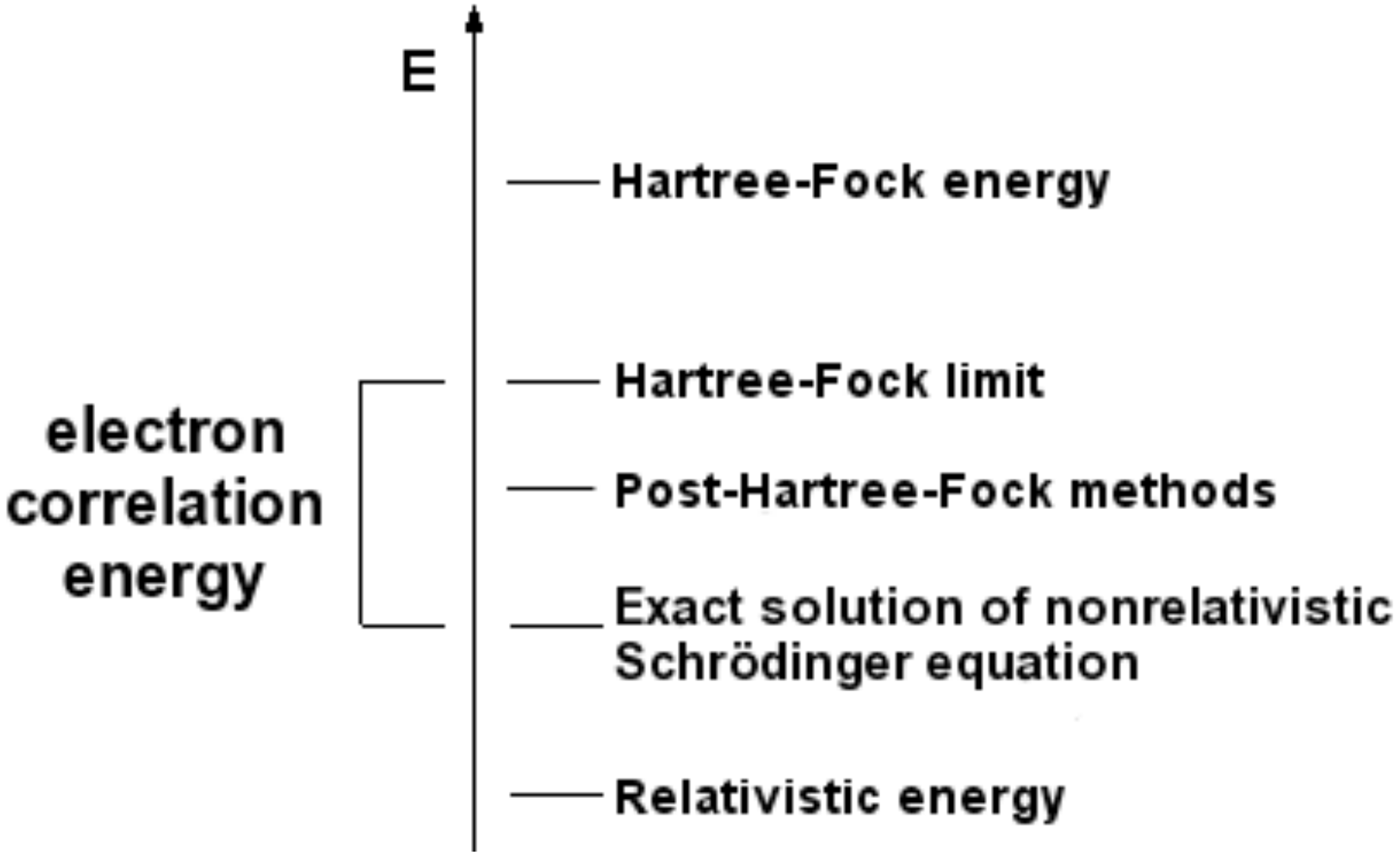
Electron correlation energy



Configuration interaction

$$|\Psi\rangle = \sum_R C_R|\Phi_R\rangle + \sum_{ai} C_{ai}|\Phi_{ai}\rangle + \sum_{ai,bj} C_{ai,bj}|\Phi_{ai,bj}\rangle$$

$$+ \sum_{ia,jb,kc} C_{ai,bj,ck}|\Phi_{ai,bj,ck}\rangle + \cdots$$

coefficients C can be calculated by solving eigenvalue problem

$$HC = EC$$

The dimension of CI space (Spin-adapted CSFs,neglect spatial symmetry) can be calculated from Weyl equation

$$D = \frac{2S+1}{m+1}\begin{pmatrix} m+1 \\ \frac{N}{2}-S \end{pmatrix}\begin{pmatrix} m+1 \\ \frac{N}{2}+S+1 \end{pmatrix}$$

CH_4, 6-31G**, 10 electron, 49 MOs. The CI dimension is

673,371,590,640

Electron correlation methods

- Truncated CI — (MR)CISD,(MR)CISDT, ….
- Cluster expansion — CCSD,CCSD(T), …..
- Multi-reference perturbation theory - CASPT2, NEVPT2
- DMRG-CI, by White, Chan, Wouter etc.
- QMC-CI by Alavi, Booth etc.

MRCISD - UC v.s. IC

Un-contracted MRCISD

$$|\Psi\rangle = \sum_R C_R|\Phi_R\rangle + \sum_{ai} C_{ai}|\Phi_{ai}\rangle + \sum_{ai,bj} C_{ai,bj}|\Phi_{ai,bj}\rangle$$

$$|\Phi_{ai}\rangle = E_{ai}|\Phi_R\rangle$$
$$|\Phi_{ai,bj}\rangle = E_{ai,bj}|\Phi_R\rangle$$

Internally contracted MRCISD

$$|\Psi\rangle = |\Psi_0\rangle + \sum_{ai} C_{ai}|\Phi'_{ai}\rangle + \sum_{ai,bj} C_{ai,bj}|\Phi'_{ai,bj}\rangle$$

$$|\Psi_0\rangle = \sum_R C_R|\Phi_R\rangle$$
$$|\Phi'_{ai}\rangle = E_{ai}|\Psi_0\rangle$$
$$|\Phi'_{ai,bj}\rangle = E_{ai,bj}|\Psi_0\rangle$$

CI matrix element

Iterative diagonalization

$$\sigma_\mu^{(n+1)} = \sum_\nu H_{\mu\nu} C_\nu$$

$$\begin{aligned} H_{\mu\nu} &= \langle \Phi_\mu | \hat{H} | \Phi_\nu \rangle \\ &= \sum_{p,q} (p|h_1|q) \Gamma_{pq} + \sum_{pr,qs} (pq|h_{12}|rs) \Gamma_{pq,rs} \end{aligned}$$

$$\Gamma_{pq}^{\mu\nu} = \langle \Phi_\mu | E_{pq} | \Phi_\nu \rangle$$

$$\Gamma_{pq,rs}^{\mu\nu} = \langle \Phi_\mu | E_{pr,qs} | \Phi_\nu \rangle$$

Coupling coefficients

$$(p|h_1|q)$$

$$(pr|h_{12}|qs)$$

Molecular integrals

Multi-electron basis

	Slater Determinate	Configuration state function
Spin adapted	NO	YES
Size	2-4 times	1
Calculation of coupling coefficients	easy	complicated

Graphic unitary group approach - GUGA

- 1950 Gelfand-Tsetlin
- 1962-1966 Biedenhavn, Moshisky, Boyu Hou
- 1974 Paldus: UGA
- 1978 Shavitt: GUGA
- 1979-1982 Schaefer, Sigbahn, Saxe, Payne
- 1984 Shepard, Lishika in Cloumbus
- 1986 - now, Wen and Wang, Xi'an-CI
- 2013 -now, Shepard, contracted GUGA

Paldus tabular, step vector and Distinct Row Table

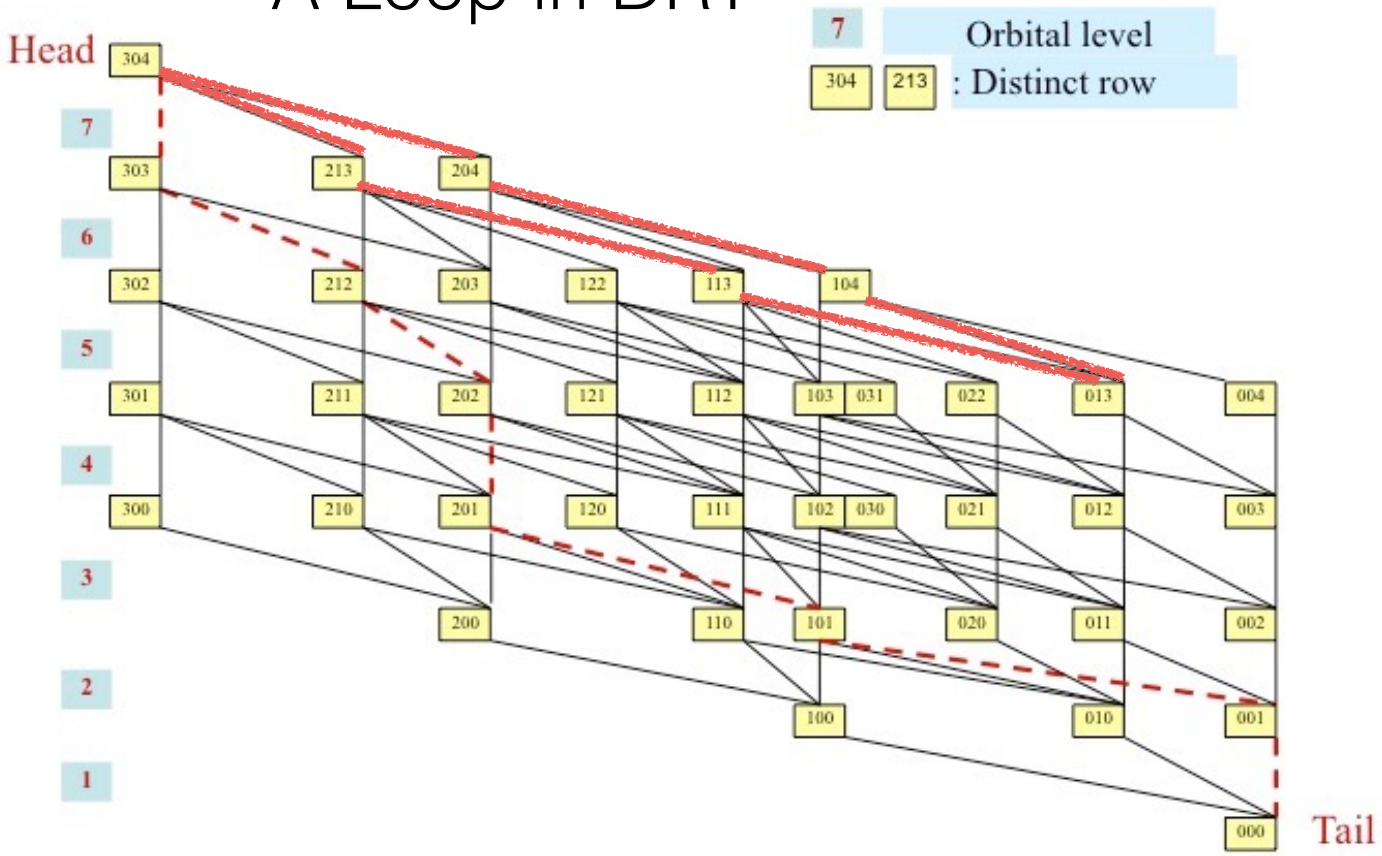
CSF is represented as Paldus tabular

$$|(abc)\rangle = \begin{vmatrix} a_n & b_n & c_n \\ \cdots & \cdots & \cdots \\ a_r & b_r & c_r \\ \cdots & \cdots & \cdots \\ a_1 & b_1 & c_1 \end{vmatrix}\rangle$$

$$|d_1 d_2 \cdots d_{n-1} d_n\rangle$$

Step vector

A Loop in DRT



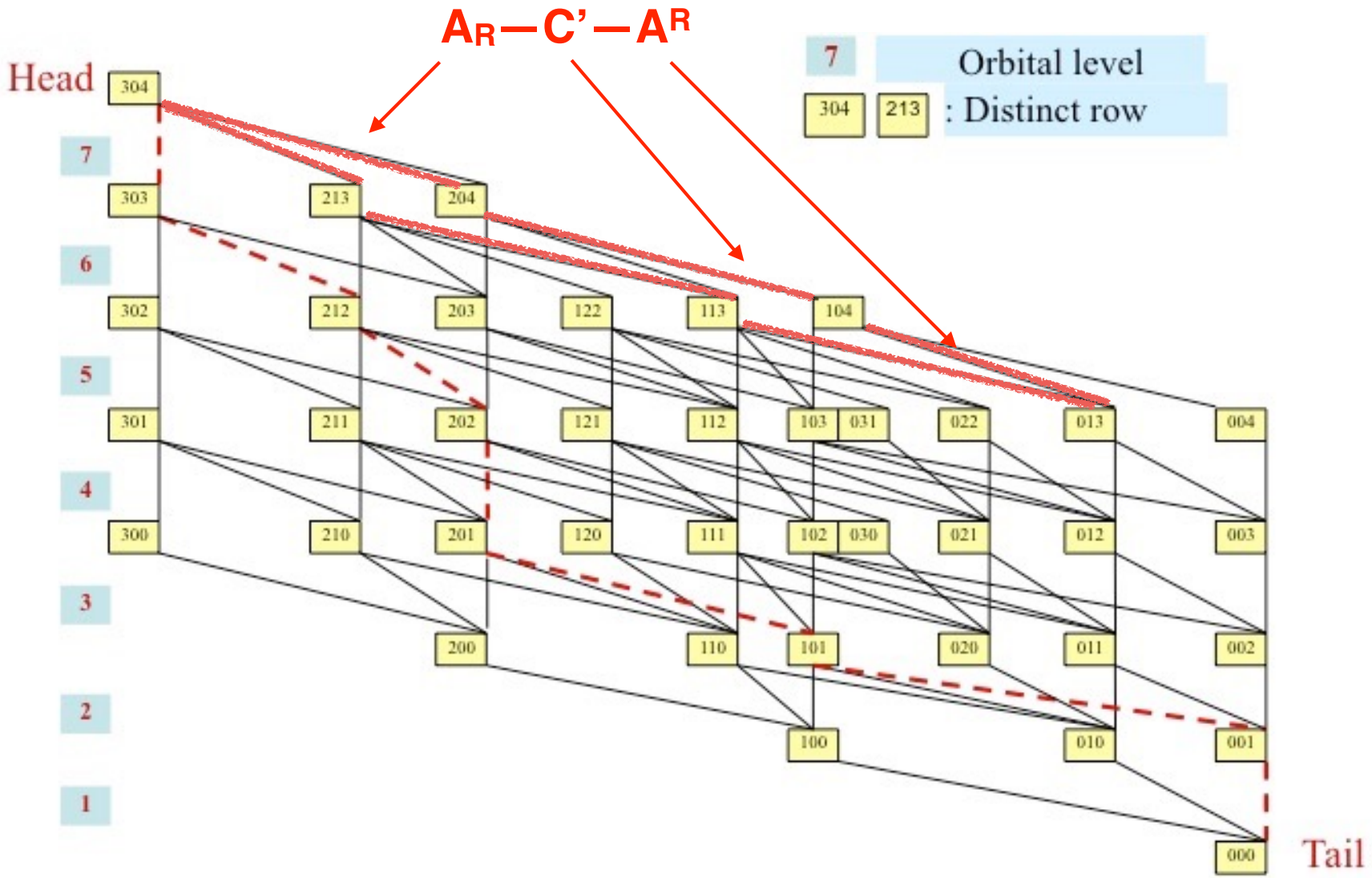
Coupling coefficients are calculated as

$$\Gamma^{\mu\nu}_{pq} = \langle d'_\mu | E_{pq} | d_\nu \rangle$$

$$= \prod_{r=min(p,q)}^{max(p,q)} W(Q_r, d'_r, d_r, \Delta b_r, b_r)$$

$$\Gamma^{\mu\nu}_{pq,rs} = \langle d'_\mu | E_{pq,rs} | d_\nu \rangle$$

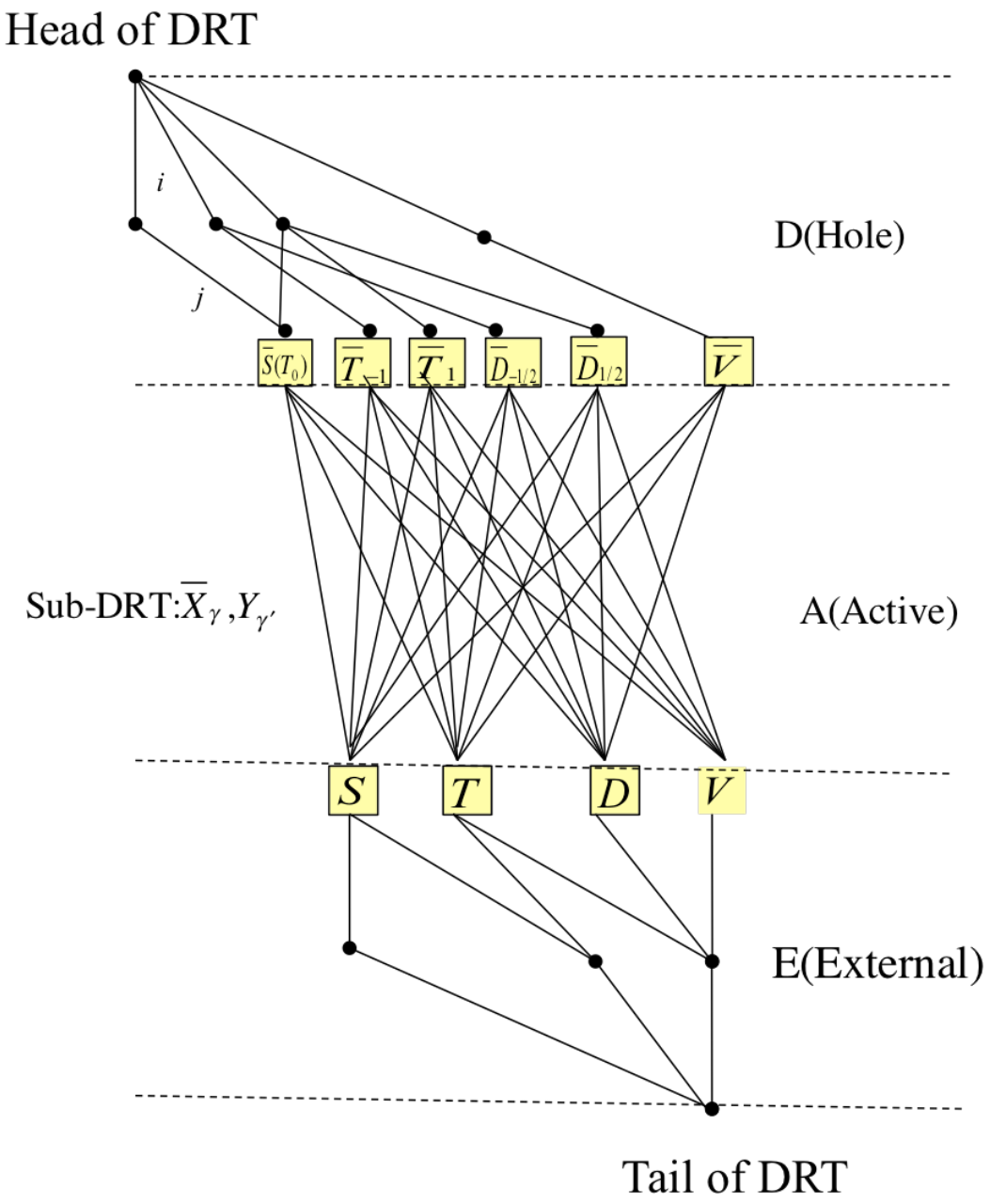
$$= \sum_{J=0,1} \omega_J \prod_{r=min(pq,rs)}^{max(pq,rs)} W(Q_r, d'_r, d_r, \Delta b_r, b_r, J)$$

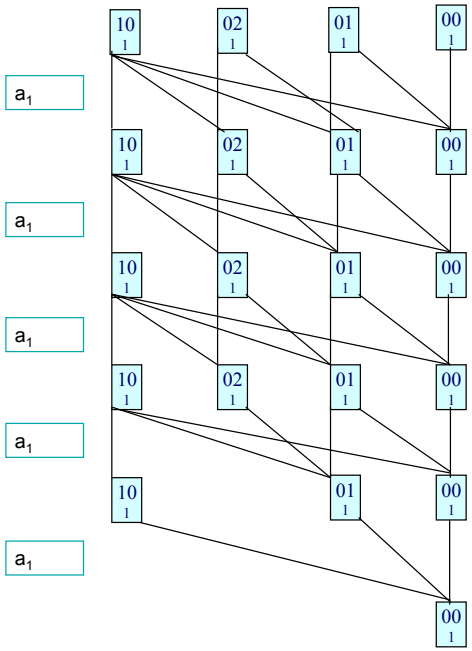


$$\Gamma^{\mu\nu}_{pq,rs} = \langle d'_\mu | E_{pq,rs} | d_\nu \rangle$$

$$= \sum_{J=0,1} \omega_J \prod_{r=min(pq,rs)}^{max(pq,rs)} W(Q_r, d'_r, d_r, \Delta b_r, b_r, J)$$

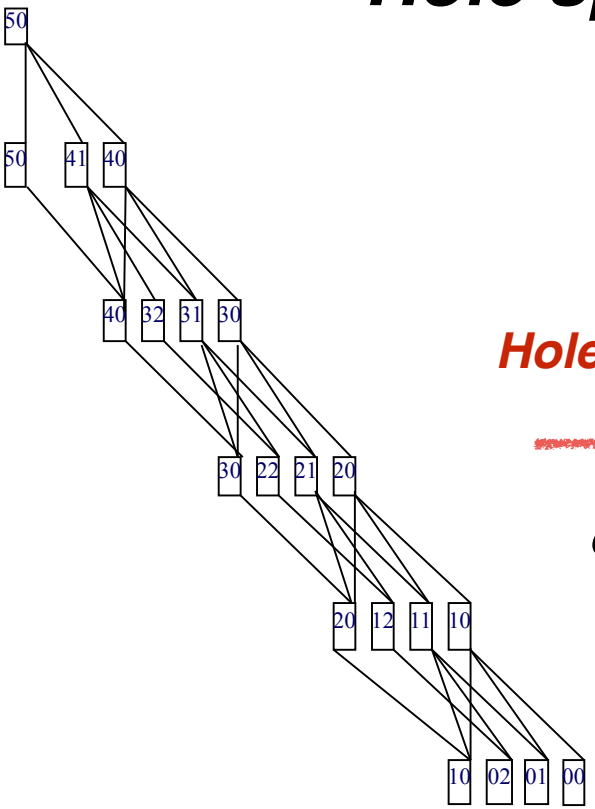
Distinct Row Table of MRCISD





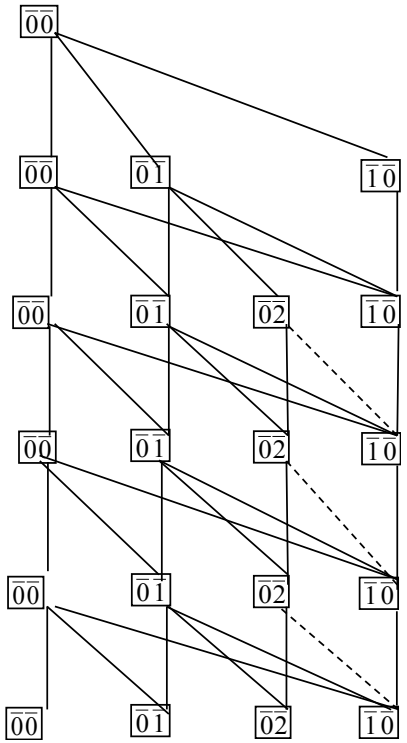
External DRT

Hole space DRT



Hole-particle trans

$$\tilde{d} = 3 - d$$



$$\Gamma_{pq}^{\mu\nu} = \langle (d')_e (d')_a (d')_h | E_{pq} | (d)_e (d)_a (d)_h \rangle$$
$$= E \cdot D \cdot A$$

$$E = \sum_{r=1}^{n_e} W(Q_r; d'_r d_r, \delta b_r, b_r)$$ **Partial Loops in external space**

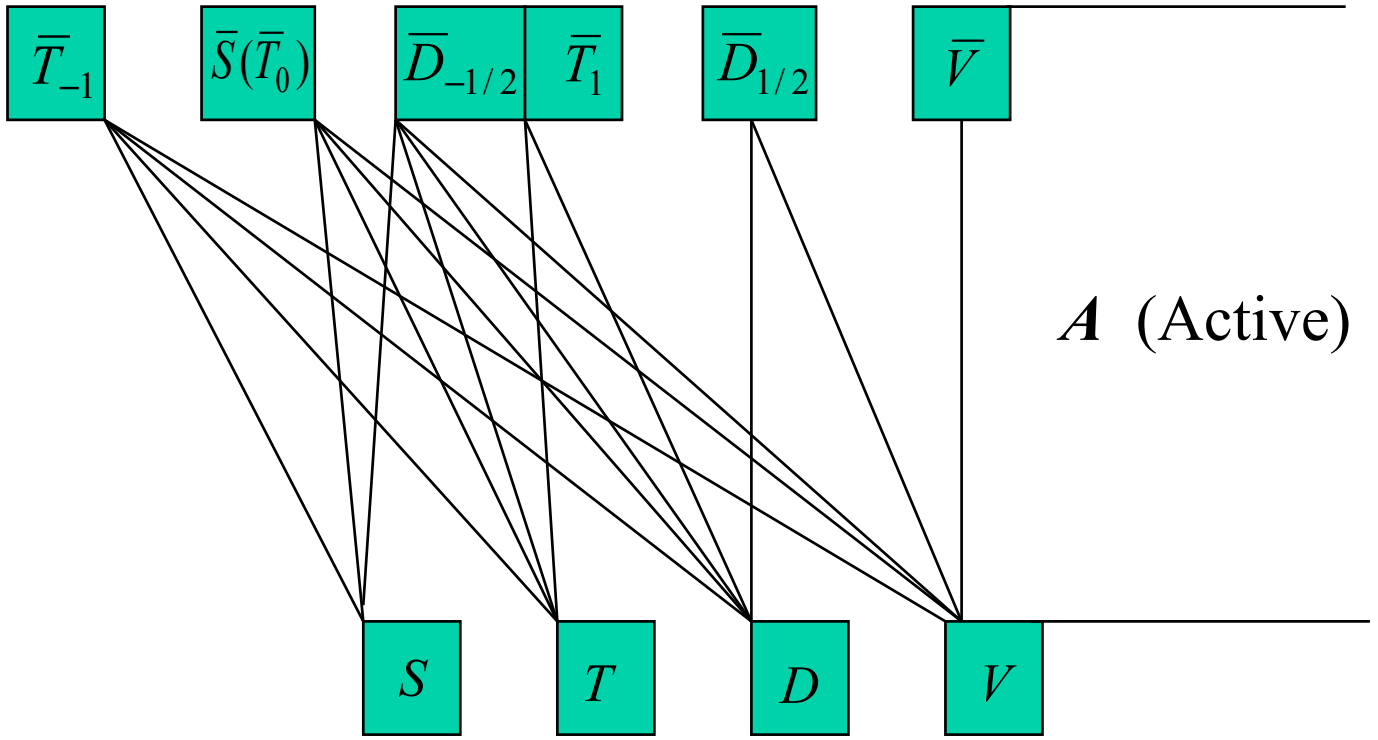
$$A = \sum_{r=n_e+1}^{n_e+n_a} W(Q_r; d'_r d_r, \delta b_r, b_r)$$ **Partial Loops in active space**

$$D = \sum_{r=n_e+n_a+1}^{n} W(Q_r; d'_r d_r, \delta b_r, b_r)$$ **Partial Loops in hole space**

E: 109 pLoop shapes
D: 244 pLoop shapes
A: Searching in active space

Programming

D (Hole)



A (Active)

E (External)

Coupling coefficient = $\boldsymbol{D \cdot A \cdot E}$

Application of Hole-particle symmetry

Molecules	**CH_2F_2**		**CH_2Cl_2**		**CH_2Br_2**	
No. orbitals	55(11+4+40)[1]		63(19+4+40)		85(37+4+44)	
Symmetry	C_{2V}					
Active space	4 electrons in orbitals: $a_1\, a_1\, b_2\, b_2$					
No. of CSFs	695,302		1,944,118		8,508,449	
	A[2]	B	A	B	A	B
No. Partial loops	1,155,011	100,756	5,122,447	100,756	33,883,641	100,756
Storage required (Kb)	51,574	3,376	231,646	3,376	1,528,500	3,376
Time per iteration (sec)[3]	39	24	176	101	1417	795

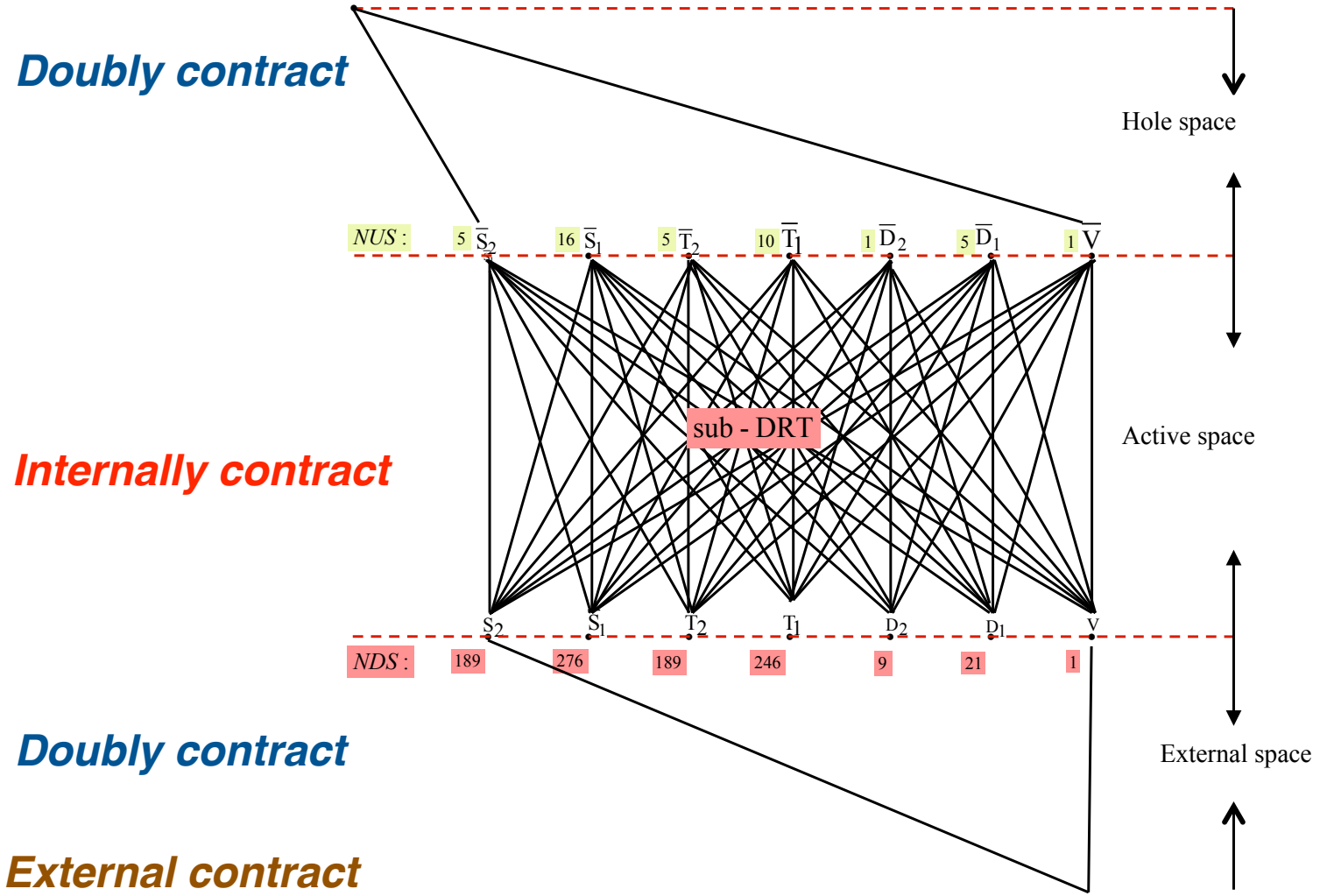
(1) In the parenthesis there are numbers of hole, active and external orbitals, respectively.

(2) A: without hole-particle symmetry; B: with hole-particle symmetry.

(3) CPU: P-4-1.6 GHz, memory: 512 Mb

Different contraction schemes based on GUGA

DRT for O_3 ()/CAS(6,6)/cc-pVDZ



$\overline{V}V$	95
$\overline{V}D_1$	108
$\overline{V}D_2$	102
$\overline{V}T_1$	49
$\overline{V}T_2$	56
$\overline{V}S_1$	57
$\overline{V}S_2$	48
$\overline{D}_1D_1$	188
$\overline{D}_1D_2$	176
$\overline{D}_1T_1$	108
$\overline{D}_1T_2$	146
$\overline{D}_1S_1$	108
$\overline{D}_1S_2$	102
$\overline{D}_2T_1$	146
$\overline{D}_2T_2$	148
$\overline{D}_2S_2$	108
$\overline{T}_1T_1$	207
$\overline{T}_2S_2$	93
$\overline{S}_1S_1$	95
$\overline{S}_2S_2$	95

icMRCI based on hole-particle symmetry

Internal contracted functions are defined ***within sub-DRTs***

$$|\Phi^{ab}_{ij;\bar{X}Y}\rangle = \hat{E}_{bj,ai}|\Phi_0\rangle$$

$$|\Phi_0\rangle = \sum_{R\in ref} c_R|\Phi_R\rangle$$

Insert an identity

$$\begin{aligned}\Psi^{ab}_{ij;\bar{X}Y} &= \sum_R c_R\hat{E}^{ab}_{ij}|\Phi_R\rangle \\ &= \sum_M |\Phi_M\rangle \sum_R c_R\langle\Phi_M|\hat{E}^{ab}_{ij}|\Phi_R\rangle \\ &= \sum_M a^M|\Phi_M\rangle\end{aligned}$$

Here

$$|\Phi_M\rangle \in \bar{X}Y \qquad a^M = \sum_R c_R\langle\Phi_M|\hat{E}^{ab}_{ij}|\Phi_R\rangle$$ ***contaction coefficient***

icMRCI based on hole-particle symmetry

$$|\Phi_M\rangle = |(d)_e(d)_a(d)_h\rangle, |\Phi_R\rangle = |(0\cdots0)_e(d)_a(3\cdots3)_h\rangle$$

Contaction coefficients can be calculated as

$$\begin{aligned} a^M &= \sum_R c_R \langle (d)_h(d)_a(d)_e|\hat{E}_{ai,bj}|(0\cdots0)_e(d)_a(3\cdots3)_h\rangle \\ &= ELS(YV)\cdot(\sum_R c_R\langle(d_\mu)_a|\hat{E}_{ai,bj}|(d_\nu)_a\rangle)\cdot HLS(\bar{X}\bar{V}) \\ &= ELS(YV)\cdot a^\mu \cdot HLS(\bar{X}\bar{V}) \end{aligned}$$

$ELS(YV)$

$HLS(\bar{X}\bar{V})$

Segment factors in external and hole space

a^μ ***is the fragment of*** a^M ***in the active space***

Test 1 - O_3 $^1A'$ (C_s) cc-pVTZ CAS(12,9)

Method	***Dimension***	***Energy(a.u.)***	Time(min)/Iters [c]
ic-MRCI (WK)[a]	2284304	-225.083654	11.24/9
ic-MRCI (WK-like)[a]	2284304	-225.083658	79.83/14
ic-MRCI (WK)[b]	6114533	-225.125812	74.22/9
ic-MRCI (WK-like)[b]	6114533	-225.125802	146.79/14
uc-MRCI(FOIS)[a]	165247124	-225.093292	2042.87/20
uc-MRCI[a]	199281704	-225.093999	2799.00/20

a 3 frozen orbital
b No frozen orbital
c Xeon x5657 3.06 GHz, 1 CPU core

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A flexible internally contracted MRCI scheme

Contraction Scheme	Contracted Sub-CI spaces	Abbrv.
Werner and Knowles	$\bar{S}(\bar{T})S(T), \bar{D}S(T), \bar{V}S(T)$	WK
SD contration	$\mathrm{WK\ contraction\ plus}\ \bar{S}(\bar{T})D$	SD
Celani and Werner	$\mathrm{SD\ contraction\ plus}\ \bar{D}D, \bar{S}(\bar{T})V$	CW
No internal excitation contraction	$\mathrm{SD\ contraction\ plus}\ \bar{D}D, \bar{V}D$	NI
Semi-full contraction	$\mathrm{CW\ contraction\ plus}\ \bar{D}V, \bar{V}D$	SFC

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CFBr calculated by different icMRCI schemes

	UC	***WK***	***SD***	***CW***	***NI***	***SFC***
	CI dimension					
$^1A'$	13,679,604,286	132,561,907	27,053,899	3,638,743	1,819,342	1,525,246
$^3A''$	27,203,671,923	246,089,715	49,661,259	7,289,103	4,046,766	3,608,930
$^1A''$	13,292,817,282	132,322,497	27,000,969	3,628,989	1,811,310	1,524,626
	Total energy (a.u.)					
$^1A'$		-0.35201711	-0.35201169	-0.35200696	-0.35196129	-0.35196114
$^3A''$		-0.30810780	-0.3080997	-0.30809192	-0.30762112	-0.30762102
$^1A''$		-0.25015951	-0.25014786	-0.25013715	-0.24897901	-0.24897896
	Relative energy (eV)					
$^1A'$		0.00	0.00	0.00	0.00	0.00
$^3A''$		1.19	1.20	1.20	1.21	1.21
$^1A''$		2.77	2.77	2.77	2.80	2.80

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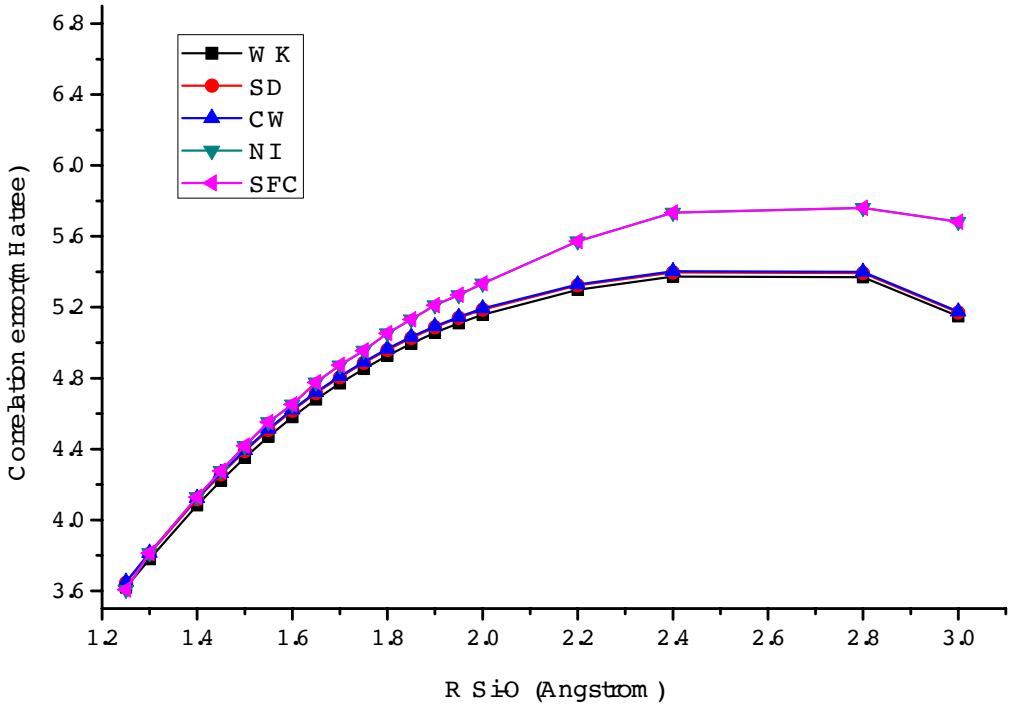
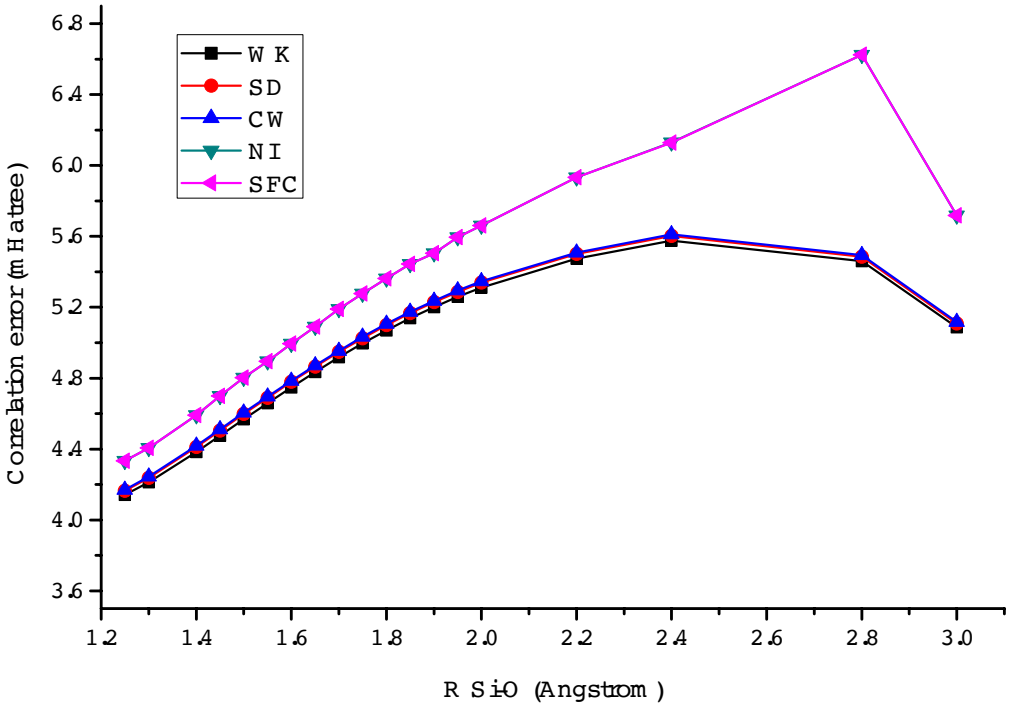
Correlation errors of PECs of SiO



$X^1\Sigma^+$



$^1\Delta$

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d-d transitions of $[Fe(H_2O)_6]^{3+}$

State	CASPT2(5,5)	CASPT2(5,10)	icMRCI(5,5)	icMRCI(5,10)	Expt.
^6A_g	0.00	0.00	0.00	0.00	0.00
$^4B_{1g}$	2.91	2.94	2.90(2.52)	2.53(2.31)	1.56
$^4B_{1g}$	3.34	3.27	3.62(3.26)	3.25(3.05)	2.29
^4A_g	3.74	3.77	3.97(3.66)	3.64(3.49)	3.01
^4A_g	3.79	3.81	4.01(3.71)	3.68(3.53)	3.05
ΔE_{abs}	0.97	0.96	1.15(0.81)	0.80(0.61)	

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Conclusion and Future development

- EN-GMFCI — treat nuclear and electron in same footing.
- icMRCI based on GUGA — much useful than un-contracted MRCI due to highly efficient.
- EN-GMF-icMRCI

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Thank you for attention!