RPA Correlation Energy at The Complete Basis Set Limit

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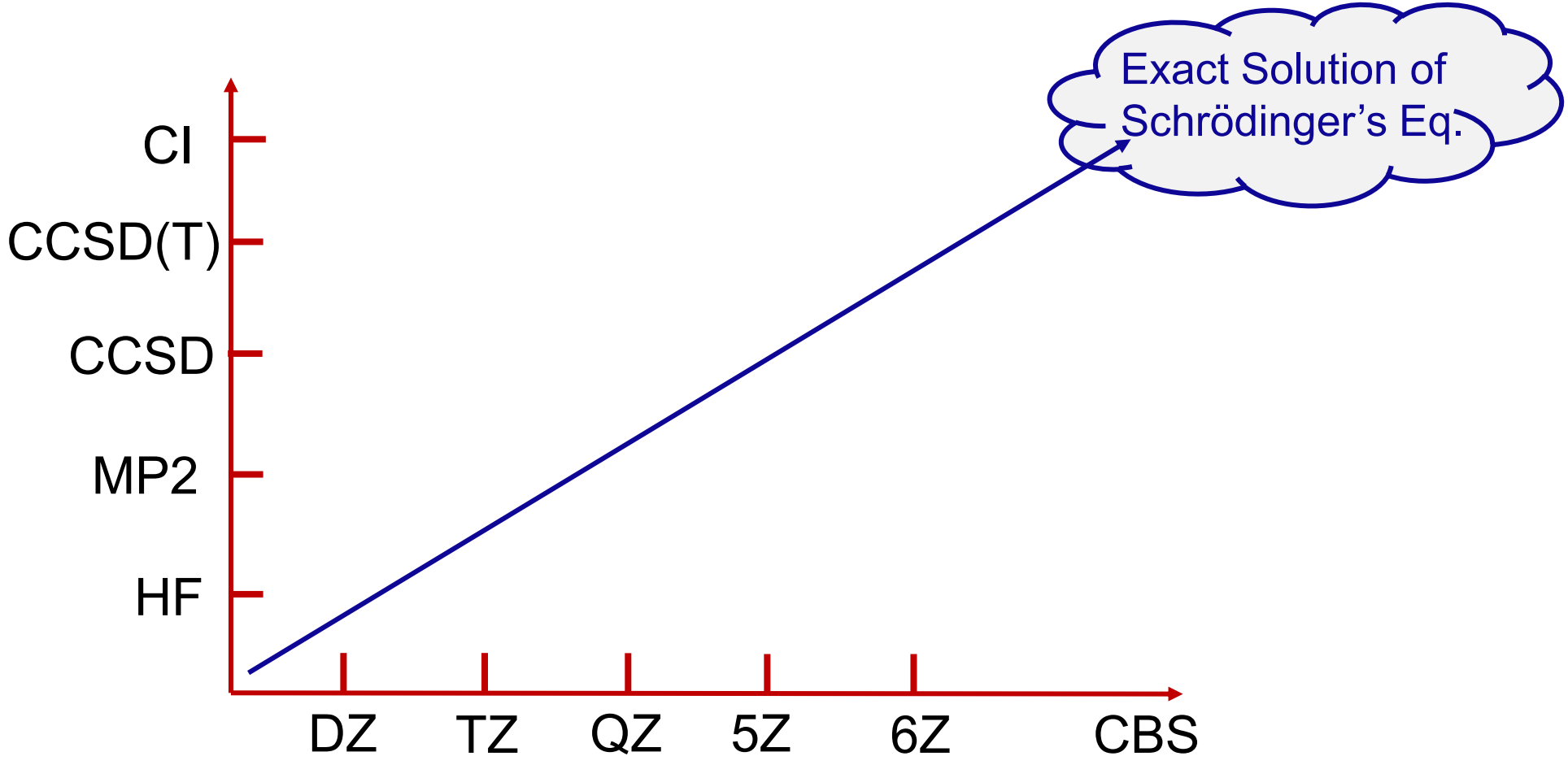
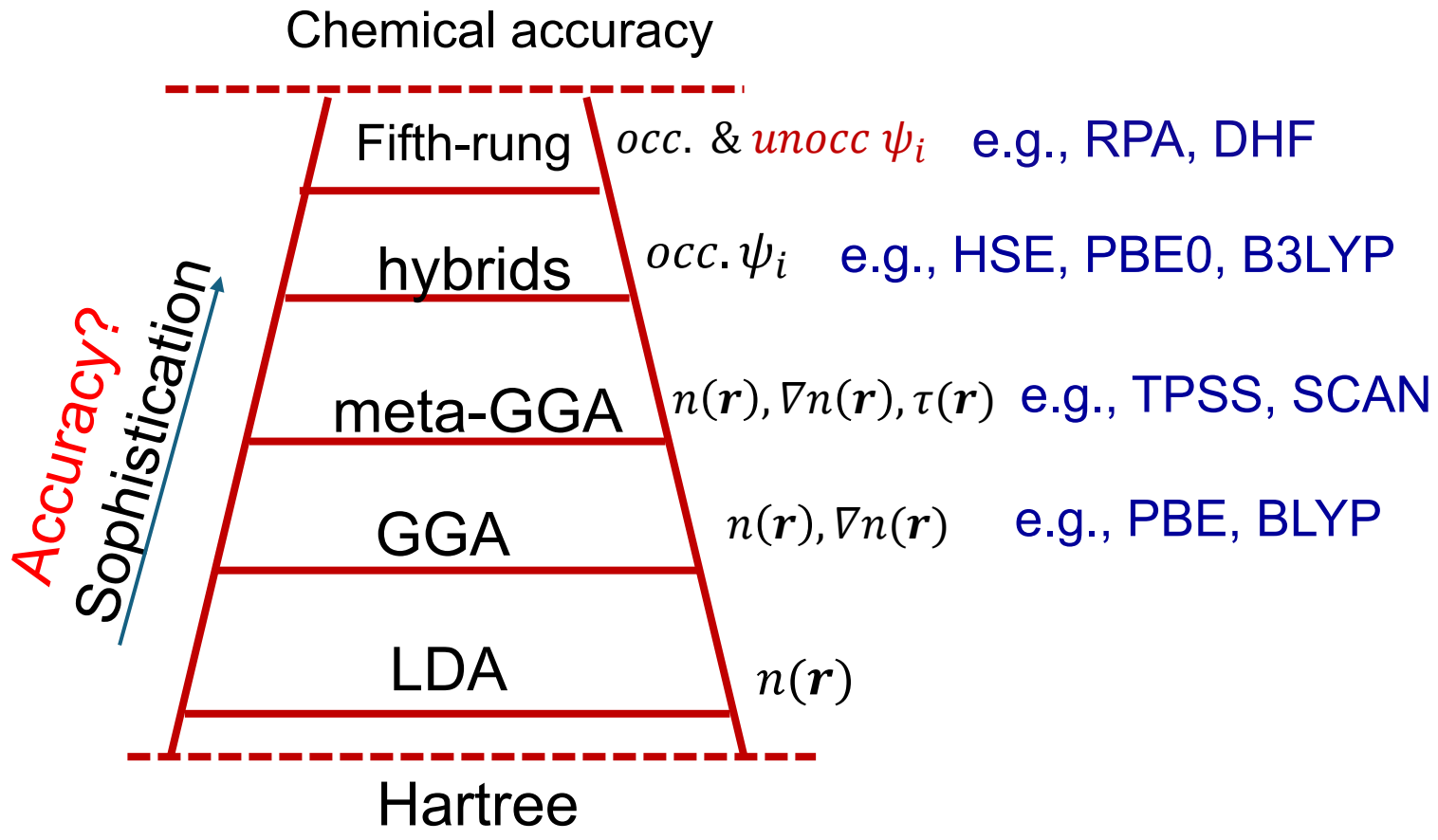
Outline

- Introduction to the random phase approximation (RPA) and the basis set issue
- Accurate RPA correlation energies by solving the Sternheimer equation on real-space grids
  - ☐ Atoms
  - ☐ Diatomic molecule
  - ☐ General polyatomic molecules
- Extension to GW
- Summary and outlook

Quantum Chemistry's Road Towards The Exact Solution of Schrödinger's Equation



Jacob's ladder in DFT



RPA has the same basis set issue as quantum chemistry methods!

J. Perdew & K. Schmidt, in Density functional theory and its application to materials, edited by Van Doren e al. (2001).

Resolution of Identity (RI) Approach to RPA

$$\chi^0(\mathbf{r},\mathbf{r}',i\omega) = 2\sum_{i,j}\frac{(f_i-f_j)\psi_i{}^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j{}^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i-\varepsilon_j-i\omega} = \sum_{\mu,\nu} P_\mu(\mathbf{r})\chi^0_{\mu\nu}(i\omega)P_\nu(\mathbf{r}')$$

$$\psi_i^*(\mathbf{r})\psi_j(\mathbf{r}) = \sum_\mu C_{ij}^\mu P_\mu(\mathbf{r})$$

$$\chi^0_{\mu\nu}(i\omega) = 2\sum_{i,j}\frac{(f_i-f_j)C_{ij}^\mu C_{ji}^\nu}{\varepsilon_i-\varepsilon_j-i\omega}$$

$$V_{\mu\nu} = \int d^3r\, d^3r' \frac{P_\mu(\mathbf{r})P_\nu(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$E_c^{\mathrm{RPA}} = \frac{1}{2\pi}\int_0^\infty d\omega\ \mathrm{Tr}[\ln(1-\chi_0(i\omega)V)+\chi_0(i\omega)V]$$

Basis set issue for RPA

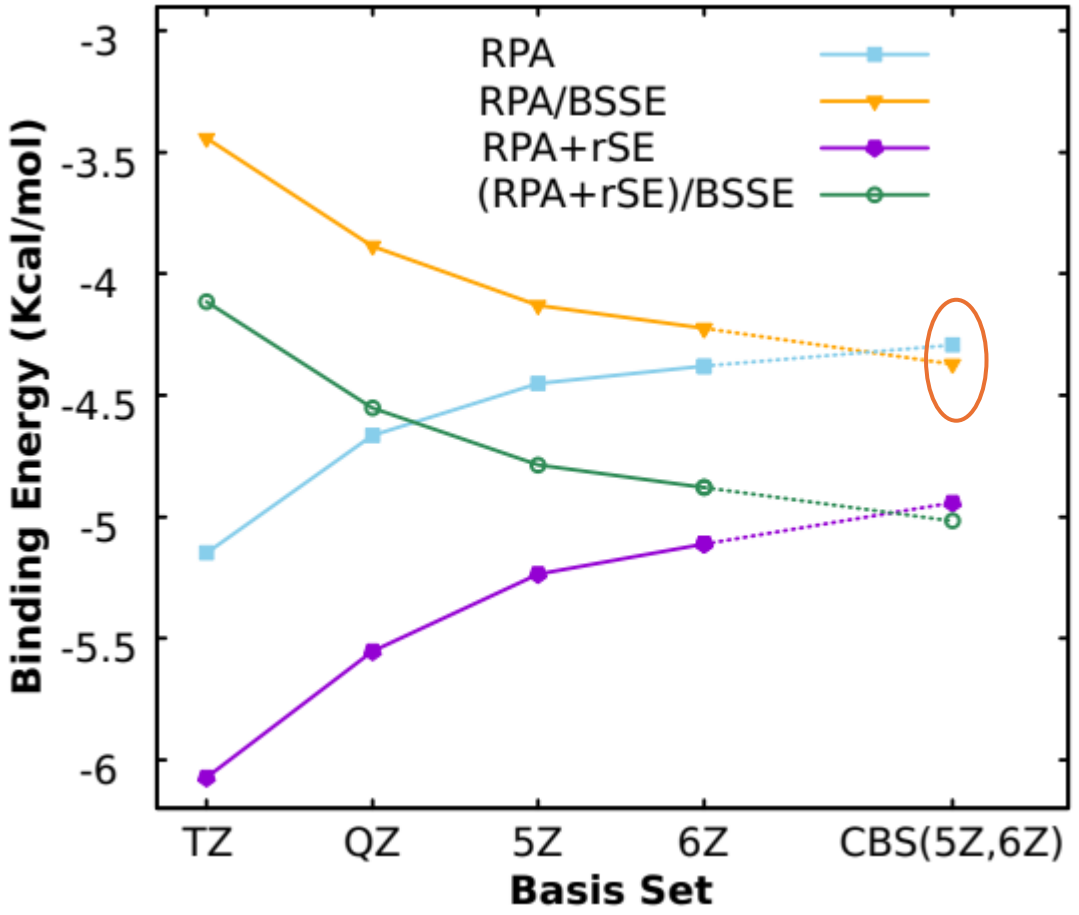
$$\chi^0(\mathbf{r},\mathbf{r}',i\omega) = 2\sum_{i,j}\frac{(f_i - f_j)\psi_i{}^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j{}^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i - \varepsilon_j - i\omega}$$

$$= 2\sum_{i}^{occ}\sum_{j}^{vir}\frac{\psi_i{}^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j{}^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i - \varepsilon_j - i\omega} + c.c.$$

- Convergence with respect to the number of unoccupied states (i.e., basis set size) is slow
- Practically one relies on converging energy differences (.e.g., binding energy) up to certain precision.
- "Correlation consistent" basis sets are preferred, which allow for extrapolation to the so-called "complete basis set" (CBS) limit.

RPA converges slow with basis size

Binding energy of the water dimer, Gaussian cc-pV*n*Z basis sets



$$E(n) = E(\infty) - \frac{\alpha}{n^3}$$

NAO basis sets: current status in the all-electron FHI-aims code

- FHI-aims-2009 ("*tier-n*") basis sets (*Blum et al., CPC 180, 2175 (2009)*) generated based on the LDA energy for dimers and suitable for ground-state DFT/HF-type calculations.

- NAO-VCC-*n*Z basis sets (*Zhang et al., NJP 15, 123033 (2013*)) generated based on RPA@PBE energy for atoms and suitable for "correlated calculations". Officially available only for H-Ar.

- "*tier-n* + aug", "*tier-n* + STO", or "*tier-n* + aug + STO" suitable for *GW* or *GW*+BSE spectroscopy calculations.

  Ren et al., NJP 14, 053020 (2012); Ren et al. PRM 5, 013807 (2021); Yao et al., JCTC 18, 1569 (2022)

Remark: Basis set requirements for RPA and *GW* are different!

RPA: Energy difference between different atomic configurations, severe BSSE
GW: Energy difference between different electronic configurations

Challenges for developing NAO-VCC-*n*Z for heavy elements

- Optimizing the RPA total energy for atoms is very inefficient for binding energy calculations.
- Frozen-core approximation has to be used, but which core to freeze is tricky. Including semi-core states lead to too big basis sets.
- The BFGS algorithm for optimization often got stuck in local minimum. One ends up with different basis sets with different “initial conditions”.
- A lot of trial and errors

Reliable CBS results are hard to obtain for heavy elements and complex systems!

Challenges for developing NAO-VCC-*n*Z for heavy elements

Is it possible to develop an approach for RPA that is free of the single-particle basis error?

- A lot of trial and errors

Reliable CBS results are hard to obtain for heavy elements and complex systems!

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Alternative formulation of density response function

$$\chi^0(\mathbf{r},\mathbf{r}',i\omega) = 2\sum_i^{occ}\sum_j^{unocc} \frac{\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i - \varepsilon_j - i\omega} + c.c.$$

Where does this expression come from?

Physically, $\chi^0(\mathbf{r},\mathbf{r}',i\omega)$ describes the linear variation of the density upon a disturbance of the Kohn-Sham effective potential,

$$\chi^0(\boldsymbol{r},\boldsymbol{r}',i\omega) = \frac{\delta n(\boldsymbol{r},i\omega)}{\delta v_{eff}(\boldsymbol{r}',i\omega)}$$

$$n(\boldsymbol{r}) = 2\sum_i^{occ}\psi_i^*(\boldsymbol{r})\psi_i(\boldsymbol{r}) \quad \Rightarrow \quad \delta n(\boldsymbol{r},i\omega) = 2\sum_i^{occ}\psi_i^*(\boldsymbol{r})\delta\psi_i(\boldsymbol{r},i\omega) + c.c.$$

First-order perturbation theory:

$$\delta\psi_i(\boldsymbol{r},i\omega) = \sum_{j\neq i}\frac{\langle\psi_j|\delta v_{eff}|\psi_i\rangle}{\varepsilon_i - \varepsilon_j - i\omega}\psi_j(\boldsymbol{r}) \quad \Rightarrow \quad \frac{\delta\psi_i(\boldsymbol{r},i\omega)}{\delta v_{eff}(\boldsymbol{r}',i\omega)} = \sum_{j\neq i}\frac{\psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')}{\varepsilon_i - \varepsilon_j - i\omega}\psi_j(\boldsymbol{r})$$

$$\frac{\delta n(\boldsymbol{r},i\omega)}{\delta v_{eff}(\boldsymbol{r}',i\omega)} = 2\sum_i^{occ}\sum_{j\neq i}\frac{\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i - \varepsilon_j - i\omega} + c.c.$$

(zero for $j \in occ$)

Alternative formulation of RI-RPA

$$\tilde{\chi}^0_{\mu\nu}(i\omega) = \iint d\boldsymbol{r}d\boldsymbol{r}'\, P_\mu(\boldsymbol{r})\chi^0(\boldsymbol{r},\boldsymbol{r}',i\omega)P_\nu(\boldsymbol{r}') = \int d\boldsymbol{r}\, P_\mu(\boldsymbol{r})n^{(1)}_\nu(\boldsymbol{r},i\omega)$$

External perturbation

Density change

$$n^{(1)}_\nu(\boldsymbol{r},i\omega) = \int d\boldsymbol{r}'\, \chi^0(\boldsymbol{r},\boldsymbol{r}',i\omega)P_\nu(\boldsymbol{r}') = \int d\boldsymbol{r}' \frac{\delta n(\boldsymbol{r},i\omega)}{\delta v_{eff}(\boldsymbol{r}',i\omega)} P_\nu(\boldsymbol{r}')$$

$\tilde{\chi}^0_{\mu\nu}(i\omega)$ can be understood as the projection of the linear density change upon a disturbance of $P_\nu(\boldsymbol{r})$ to a function $P_\mu(\boldsymbol{r})$.

$$\chi_{\mu\nu}(i\omega) = \sum_{\mu',\nu'} S^{-1}_{\mu\mu'}\, \tilde{\chi}^0_{\mu'\nu'}(i\omega) S^{-1}_{\nu'\nu} \qquad S_{\mu\nu} = \int d\boldsymbol{r}\, P_\mu(\boldsymbol{r})P_\nu(\boldsymbol{r})$$

How to determine first-order density $n^{(1)}_\nu(\boldsymbol{r},i\omega)$?

- Expanding $n^{(1)}_\nu(\boldsymbol{r},i\omega)$ in terms of the eigenspectrum of $\hat{H}_{KS}$ ➔ “Sum of States approach”.
- Directly calculating $n^{(1)}_\nu(\boldsymbol{r},i\omega)$ by solving a differential equation.

In practice, directly determine the spectra of $\chi^0 v$

$$\chi^0 v|\phi_n\rangle = e_n|\phi_n\rangle$$

Iteratively determine the eigenspectrum of the $\chi^0 v$ operator!

$$\langle \boldsymbol{r}|v|\phi_n\rangle = \int \frac{\phi_n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} dr' = \tilde{\phi}_n^v(\boldsymbol{r})$$

Solving the Poisson Eq.

$$\langle \boldsymbol{r}|\chi^0|\tilde{\phi}_n^v\rangle = \delta n(\boldsymbol{r})$$

Solving the Sternheimer Eq.

The Sternheimer equation approach

$$n^{(1)}(\boldsymbol{r}, i\omega) = \delta n(\boldsymbol{r}, i\omega) = 2\sum_{i}^{occ} \psi_i^*(\boldsymbol{r})\, \psi_i^{(1)}(\boldsymbol{r}, i\omega) + c.c.$$

$\psi_m^{(1)}(\boldsymbol{r}, i\omega)$ satisfies the so-called Sternheimer equation:

$$\left[H^{(0)} - E_i^{(0)} + i\omega\right] \psi_i^{(1)}(\boldsymbol{r}, i\omega) = \left[E_i^{(1)} - V^{(1)}\right] \psi_i^{(0)}(\boldsymbol{r})$$

where

$$H^{(0)}\psi_i^{(0)}(\boldsymbol{r}) = E_i^{(0)}\psi_i^{(0)}(\boldsymbol{r})$$

$$E_i^{(1)} = \left\langle \psi_i^{(0)} \middle| V^{(1)} \middle| \psi_i^{(0)} \right\rangle \qquad V^{(1)}(\boldsymbol{r}) = P_v(\boldsymbol{r})$$

- Expanding $\psi_i^{(1)}(\boldsymbol{r}, i\omega)$ in terms of atomic orbital basis yields the same results as the "sum over states" approach.
- Solving the Sternheimer equation on a real-space grid can go beyond the Hilbert space expanded by the finite NAO basis set.

Solving the Sternheimer equation for a single atom

Simplifications for a single atom:

$$\psi_i^{(0)}(\boldsymbol{r}) = u_{il}^{(0)}(r) Y_{lm}(\theta, \varphi)$$

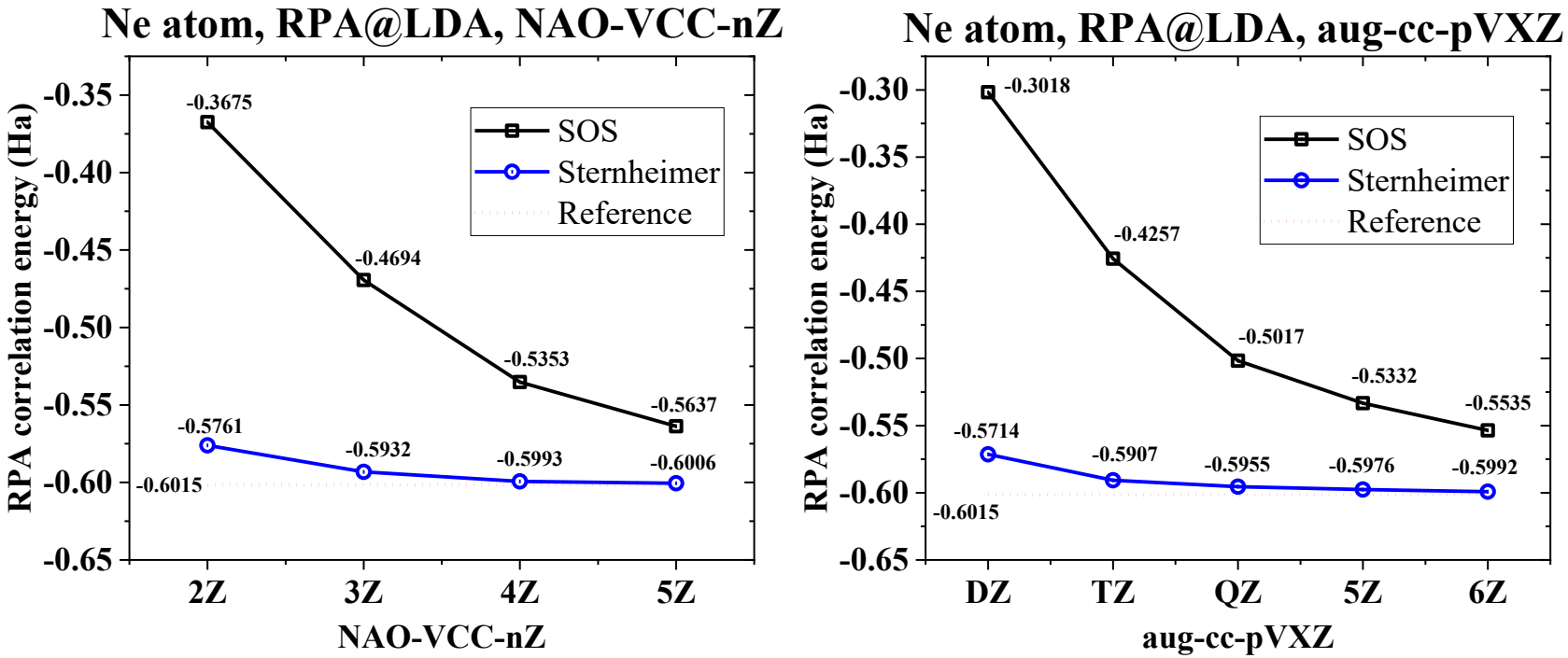
$$\psi_i^{(1)}(\boldsymbol{r}, i\omega) = \sum_{l'm'} u_{i,l'm'}^{(1)}(r, i\omega) Y_{l'm'}(\theta, \varphi)$$

$$V^{(1)}(\boldsymbol{r}) = P_v(\boldsymbol{r}) = V^{(1)}(r) Y_{LM}(\theta, \varphi)$$

$$\left(-\frac{1}{2r}\frac{\partial^2}{\partial r^2} r + \frac{l'(l'+1)}{2r^2} + V(r) - E_i^{(0)} + i\omega\right) u_{i,l'm'}^{(1)}(r, i\omega)$$
$$= G_{l'Ll}^{m'Mm}\left(E^{(1)}\delta_{l',l}\delta_{m',m} - V^{(1)}(r)\right) u_{il}^{(0)}(r)$$

The Sternheimer equation is reduced to a one-dimensional radial differential equation that can be solved by the finite difference method on a dense radial grid.

Basis set convergence for the RPA correlation energy



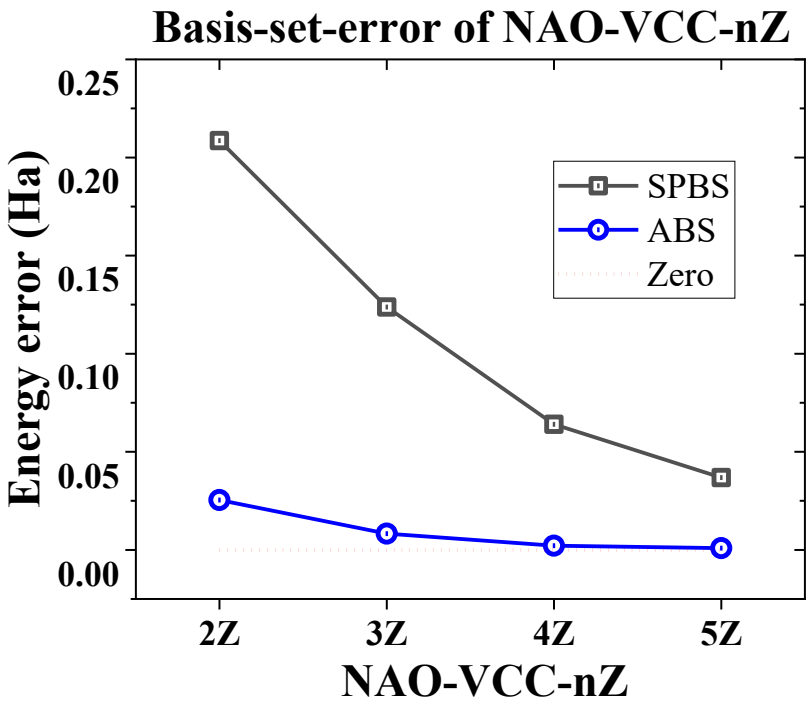
The Sternheimer results still depends on the auxiliary (RI) basis sets generated by the single particle orbitals.

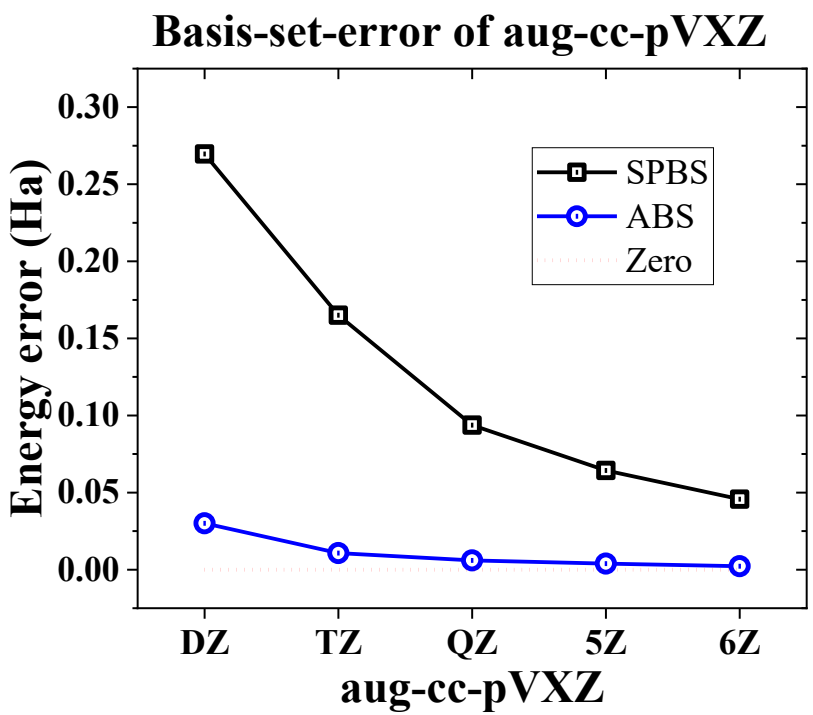
Reference results are obtained using the "hard-wall cavity" method:

Jiang & Engel, JCP 127, 184108 (2007)

Distinguishing SPBS errors and RI errors

SPBS: single-particle basis set; ABS: auxiliary basis set set

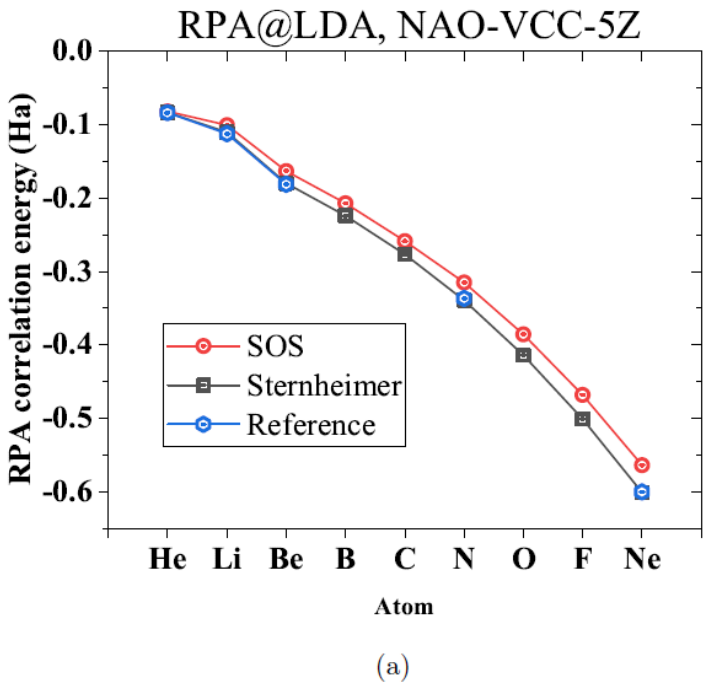




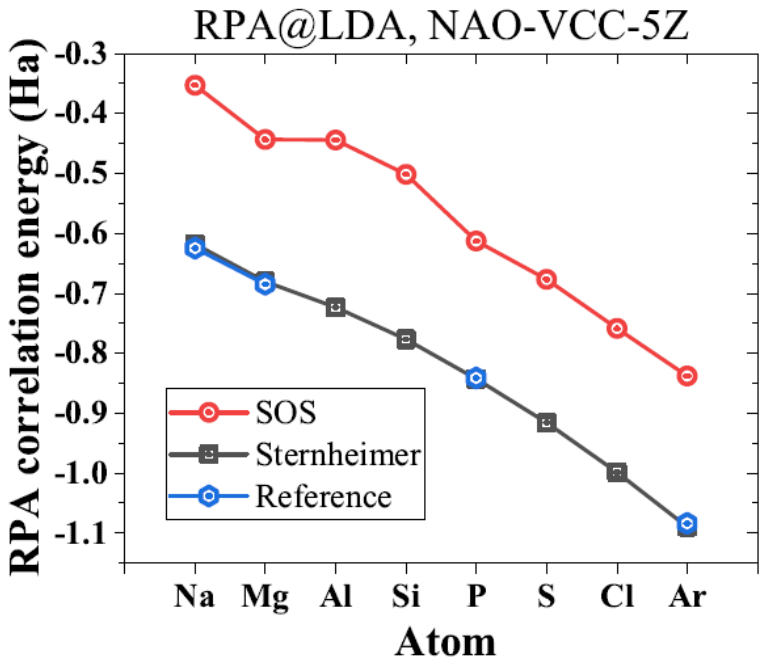
$$\Delta^{(1)}\chi^0(\mathbf{r},\mathbf{r}',i\omega) = \chi^0(\mathbf{r},\mathbf{r}',i\omega) - \left(2\sum_i^{occ}\sum_j^{unocc}\frac{\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')}{\varepsilon_i-\varepsilon_j-i\omega}+c.c.\right)$$: SPBS error

$$\Delta^{(2)}\chi^0(\mathbf{r},\mathbf{r}',i\omega) = \chi^0(\mathbf{r},\mathbf{r}',i\omega) - \left(\sum_{\mu,\nu}P_\mu(\mathbf{r})\,\chi^0_{\mu\nu}(i\omega)P_\nu(\mathbf{r}')\right)$$: RI error

RPA correlation energies for other atoms



(a)

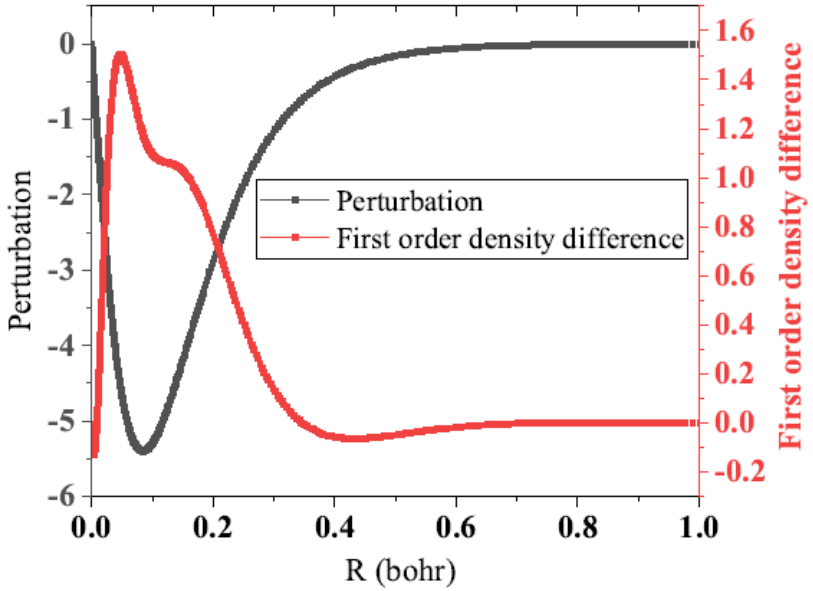


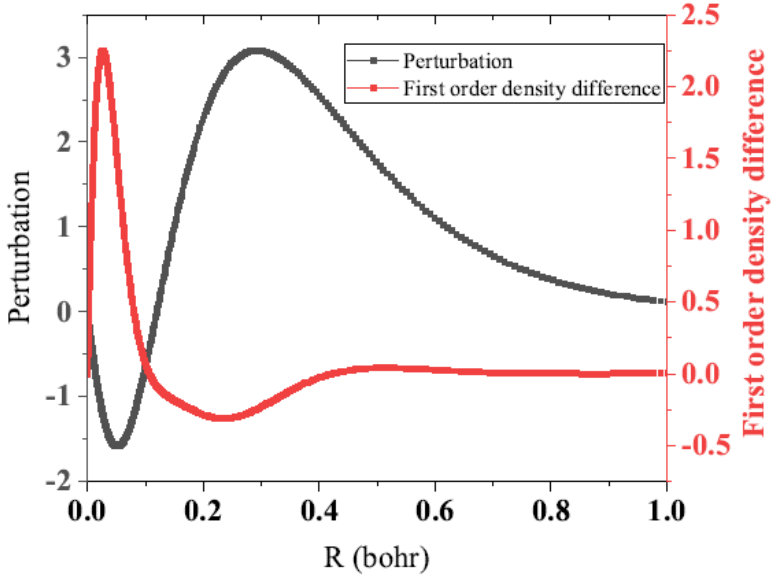
Accurate RPA correlation energies for atoms from H to Kr are provided.

H. Peng, S. Yang, H. Jiang, H., Weng, and X. Ren, J. Chem. Theory Comput. **19**, 7199 (2023).

Visualizing the basis set error in real space

$$\delta n^{(1)}(r) = n^{(1)}_{\text{Sternheimer}} - n^{(1)}_{\text{SOS}}$$





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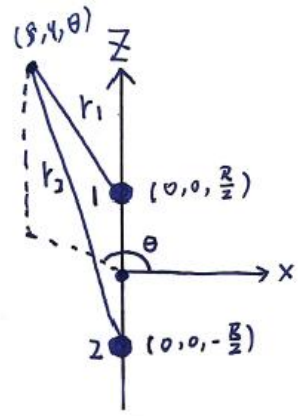
Solving the Sternheimer equation for diatomic molecules



The prolate spheroidal coordinates system （长球面坐标系）

$$\xi = \frac{r_1 + r_2}{2}, \qquad 0 \le \xi < \infty$$

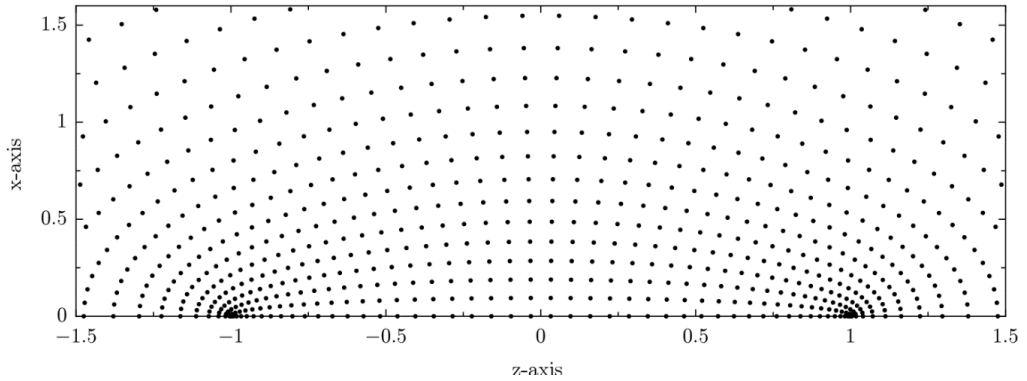
$$\eta = \frac{r_1 - r_2}{R}, \quad -1 \le \eta \le 1$$

θ: azimuth angle, $0 \le \theta \le 2\pi$

For convenience, transforming prolate spheroidal coordinates (ξ, η, θ) are transformed into (μ, ν, θ) variables:

$$\mu = cosh^{-1}\xi \quad 0 \le \mu \le \infty$$
$$\upsilon = cos^{-1}\eta \quad 0 \le \upsilon \le \pi$$

$$N_\mu = 120\sim180$$
$$N_\upsilon = 100\sim150$$
$$\mu(i) = (i-1) * h_\mu$$
$$\upsilon(i) = (i-1) * h_\upsilon$$



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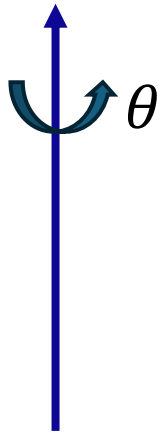
$$\left[H^{(0)} - E_i^{(0)} + i\omega\right]\psi_i^{(1)}(\boldsymbol{r}, i\omega) = \left[E_i^{(1)} - V^{(1)}\right]\psi_i^{(0)}(\boldsymbol{r})$$



$$\psi_i(\boldsymbol{r}) = f(\mu, \nu)e^{im\theta}$$

$$V^{(1)}(\boldsymbol{r}) = V^{(1)}(\mu, \nu)e^{iM\theta}$$

$$\psi_i^{(1)}(\boldsymbol{r}, i\omega) = f_{m+M}^{(1)}(\mu, \nu)e^{i(m+M)\theta}$$

For each M, solve a set of linear equation on grids (μ, ν)

Convergence parameters:

Grid size: (N_μ, N_ν)
Maximal M : $M_{\max}$
Number of eigenmodes: N_{eigen}
Number of frequency points: N_ω

RPA correlation energy

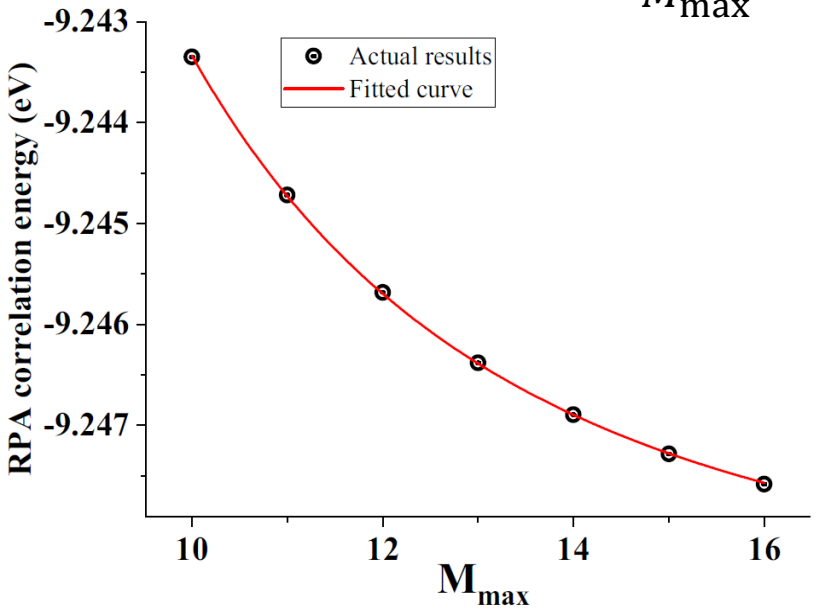
$$E_{\text{c}}^{\text{RPA}} = \frac{1}{2\pi}\int d\omega \sum_{M}^{M_{\max}} \sum_{i}^{N_{\text{eigen}}} \left[\ln\left(1 - e_{i,M}(\text{i}\omega)\right) + e_{i,M}(\text{i}\omega)\right]$$

Convergence behavior

Convergence with respect to N_{eigen}

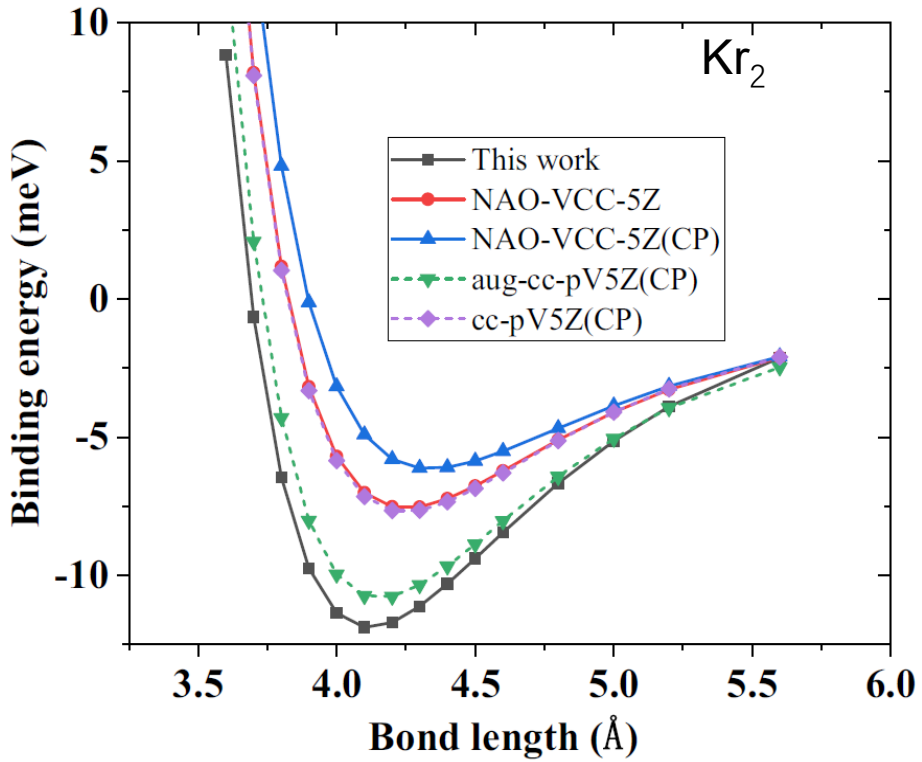
N_{eigen}	$E_c^{\mathrm{RPA}}(\mathrm{N_2})$	$E_c^{\mathrm{RPA}}(\mathrm{N})$	$\Delta E_c^{\mathrm{RPA}}$
100	–23.36237	–9.22194	–4.91849
200	–23.38841	–9.23521	–4.91800
300	–23.39446	–9.23829	–4.91789
400	–23.39687	–9.23951	–4.91785
500	–23.39808	–9.24013	–4.91782
600	–23.39879	–9.24049	–4.91781
700	–23.39923	–9.24071	–4.91780
800	–23.39954	–9.24087	–4.91780
900	–23.39975	–9.24098	–4.91779
1000	–23.39990	–9.24106	–4.91778

$$E(M_{\mathrm{max}}) = E(\infty) + \frac{\alpha}{M_{\mathrm{max}}^3}$$

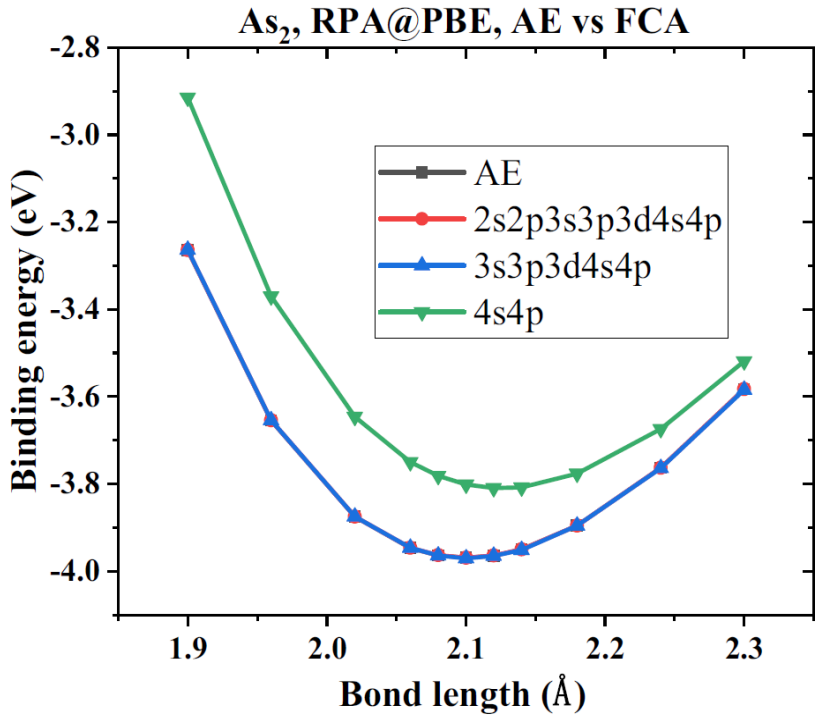


*H. Peng and X. Ren, Phys. Rev. A **112**, 062819 (2025)*

Test results for dimers



Error of frozen-core approximation



Benchmark results for diatomic molecules

F12方法

Molecule	Bond length	This work	NAO[CBS(4,5)]	GTO[cc-pV6Z]	GTO[CBS(5,6)]	Ref. [10]
H_2	0.74	108.72	108.72(0.00)	108.68(−0.04)	108.77(0.05)	108.69(−0.03)
He_2	4.30	0.001	−0.001(−0.002)	0.001(0.000)	0.001(0.000)	/
Li_2	2.70	18.84	18.85(0.01)	18.50(−0.34)*	18.75(−0.09)*	18.91(0.07)
N_2	1.10	223.31	222.68(−0.63)	221.50(-1.81)	223.20(−0.11)	223.34(0.03)
F_2	1.43	30.58	30.61(0.03)	29.69(−0.89)	30.50(−0.08)	30.56(−0.02)
LiH	1.60	54.65	54.63(−0.02)	53.77(−0.88)*	54.39(−0.26)*	54.48(−0.17)
HF	0.92	132.60	132.47(−0.13)	131.84(−0.76)	132.76(0.16)	132.59(−0.01)
LiF	1.58	127.25	127.02(−0.23)	124.20(-3.05)*	126.64(−0.61)*	127.20(−0.05)
CO	1.14	244.47	244.07(−0.40)	242.95(-1.52)	244.26(−0.21)	244.46(−0.01)
Ne_2	3.24	0.041	−0.006(−0.047)	0.025(−0.016)	0.030(−0.011)	/
Na_2	3.18	13.24	13.04(−0.20)	12.93(−0.31)*	13.26(0.02)*	/
K_2	4.14	9.06	/	/	/	/
Rb_2	4.50	8.21	/	/	/	/
P_2	1.91	115.96	115.18(−0.78)	113.62(−2.34)	115.13(−0.83)	/
As_2	2.06	86.48	/	83.98(−2.50)*	85.96(−0.52)*	/
Cl_2	2.02	49.76	48.92(−0.84)	48.32(-1.44)	49.57(−0.19)	/
Ar_2	3.84	0.200	0.077(−0.123)	0.182(−0.018)	0.199(−0.001)	/
Br_2	2.24	40.67	/	38.32(−2.35)*	39.99(−0.68)*	/
I_2	2.65	84.72	/	/	/	/

H. Peng and X. Ren, Phys. Rev. A ***112****, 062819 (2025)*

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Solving the 3D Sternheimer Equation

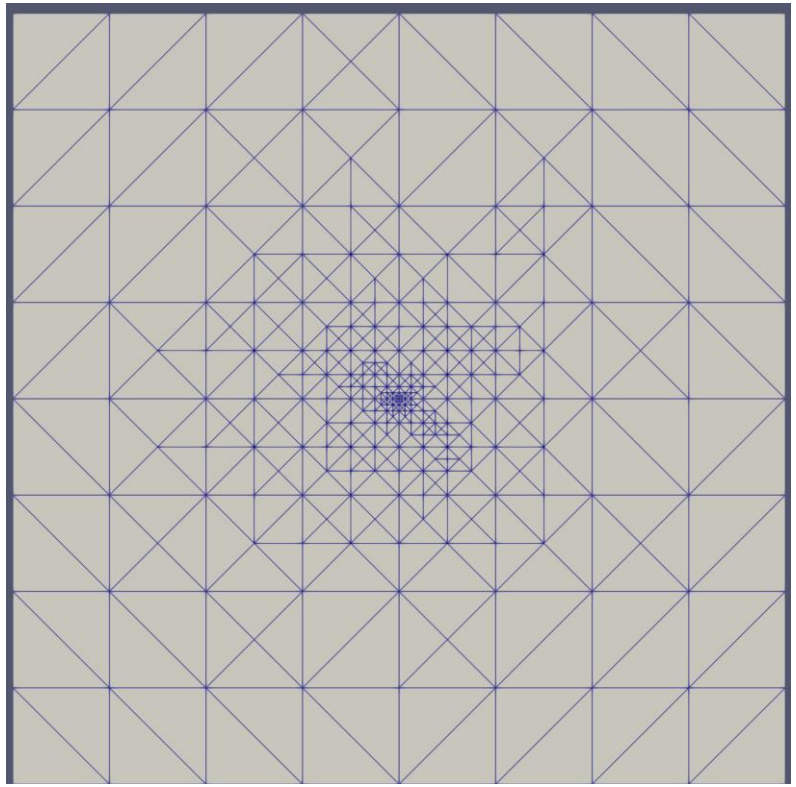
A Delta-Sternheimer Approach combining NAOs and finite element grids

$$\psi_i^{(1)}(\boldsymbol{r}, i\omega) = \psi_{i,\mathrm{out}}^{(1)}(\boldsymbol{r}, i\omega) + \psi_{i,\mathrm{in}}^{(1)}(\boldsymbol{r}, i\omega).$$

FE space AO space

$$H^{(0)}|\psi_{a,\mathrm{AO}}\rangle = \epsilon_{a,\mathrm{AO}}|\psi_{a,\mathrm{AO}}\rangle + |D_a\rangle$$

$$\psi_i^{(1)}(\mathbf{r}, i\omega) = \psi_{i,\mathrm{out}}^{(1)}(\mathbf{r}, i\omega) + \sum_a^{N_{\mathrm{unocc}}} \left(\frac{\langle \psi_{a,\mathrm{AO}} | V^{(1)} | \psi_i \rangle}{\epsilon_i - \epsilon_{a,\mathrm{AO}} - i\omega} + \frac{\left\langle D_a \middle| \psi_{i,\mathrm{out}}^{(1)}(i\omega) \right\rangle}{\epsilon_i - \epsilon_{a,\mathrm{AO}} - i\omega} \right) \psi_{a,\mathrm{AO}}(\mathbf{r}).$$



Finite Element (FE) Grid

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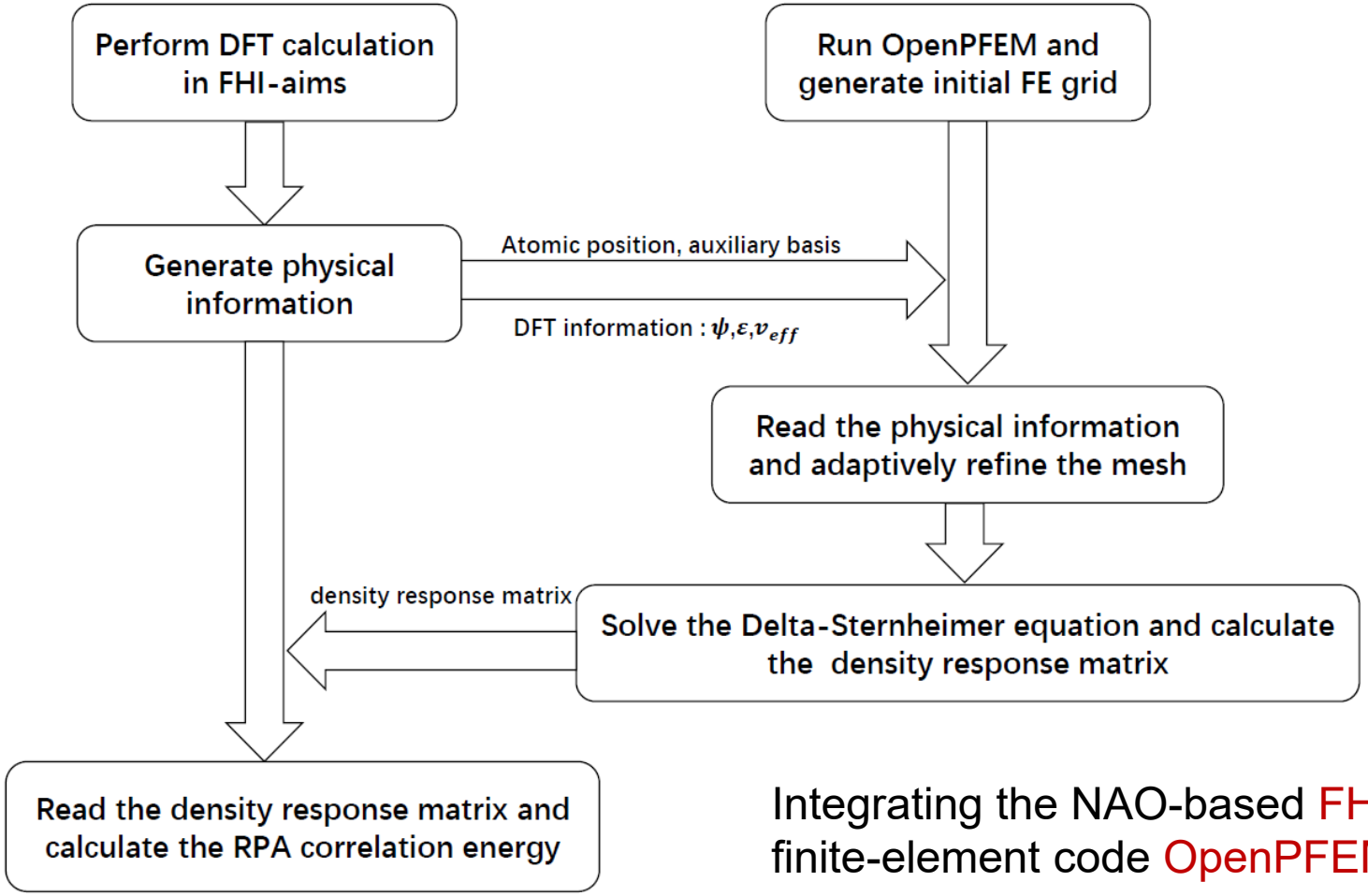
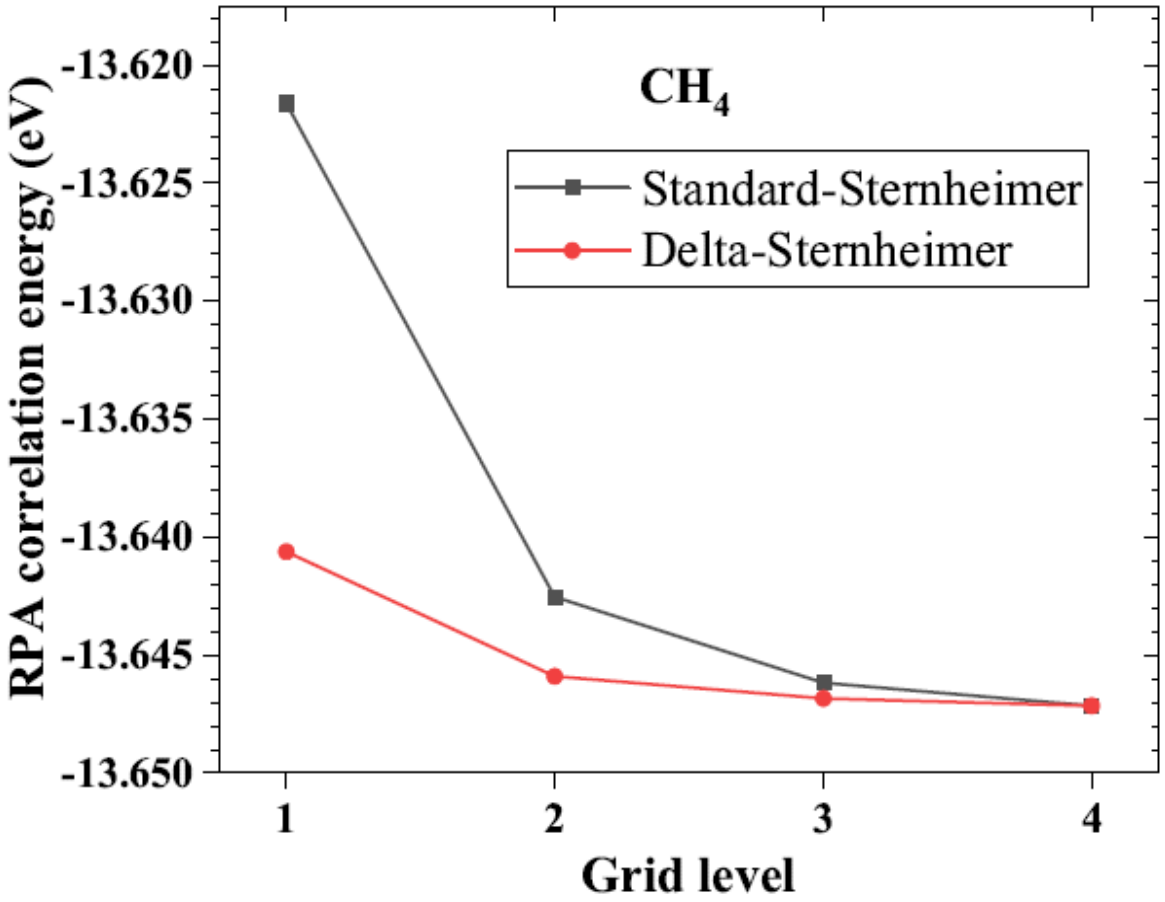
Workflow of the Delta-Sternheimer Approach



Integrating the NAO-based FHI-aims code and the finite-element code OpenPFEM.

Convergence behavior with the FE grid density



Grid Level	NOF
1	94159
2	123074
3	182006
4	238577

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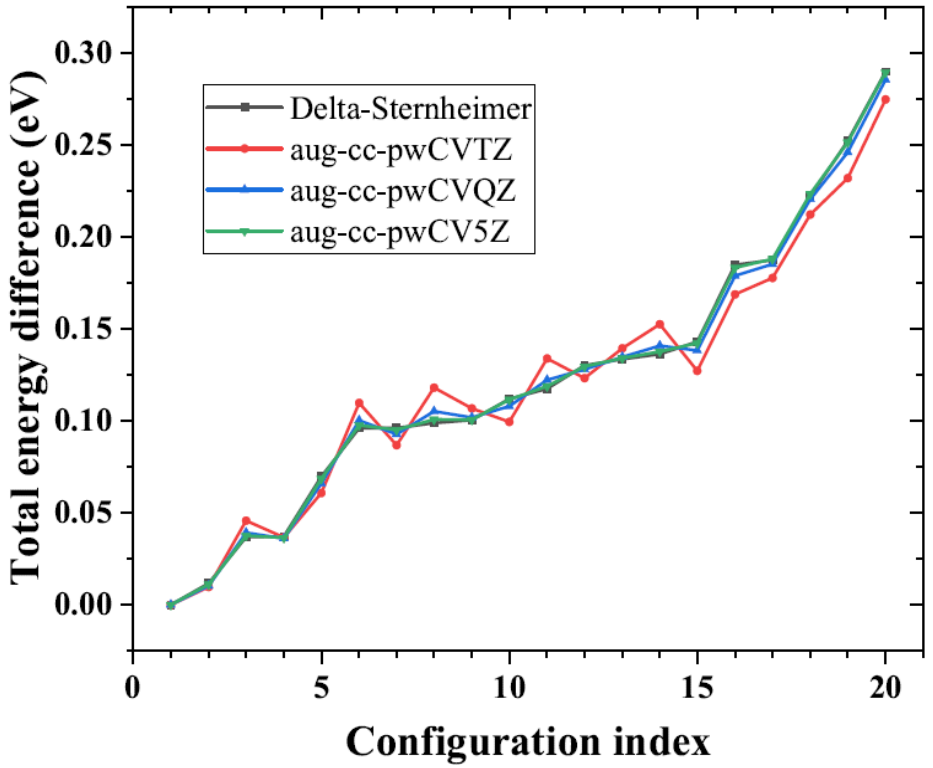
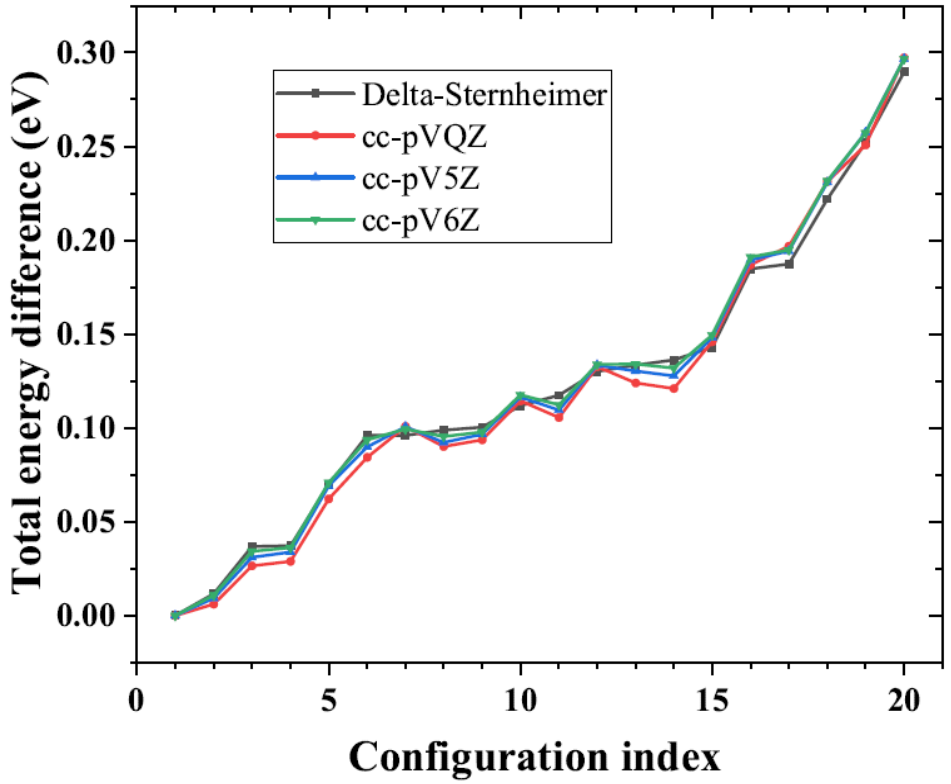
Energy hierarchy of 20 water dimer configurations





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Basis error in atomization energies

5Z: aug-pwCV5Z **CBS(Q,5)** **Unit: kcal/mol**

Molecule	5Z (CP)	5Z	Extra (CP)	Extra	This work
H_2O	-221.80 (1.77)	-222.99 (0.58)	-223.58 (-0.01)	-223.90 (-0.33)	-223.57
NH_3	-289.17 (2.13)	-290.54 (0.76)	-291.29 (0.00)	-291.59 (-0.29)	-291.30
CO_2	-362.38 (4.06)	-364.59 (1.85)	-366.49 (-0.05)	-366.76 (-0.32)	-366.44
CH_2O	-353.93 (3.03)	-355.69 (1.27)	-356.89 (0.07)	-357.17 (-0.21)	-356.97
C_2H_6	-681.87 (4.24)	-684.54 (1.57)	-686.04 (0.08)	-686.51 (-0.40)	-686.11
C_3H_6-2	-810.44 (5.88)	-815.37 (0.95)	-816.20 (0.12)	-816.75 (-0.43)	-816.32
C_2NH_3	-584.71 (5.17)	-587.85 (2.02)	-589.83 (0.05)	-590.30 (-0.42)	-589.88
SiH_4	-314.21 (2.06)	-316.10 (0.17)	-315.98 (0.29)	-316.57 (-0.30)	-316.27
PH_3	-237.47 (1.92)	-239.30 (0.08)	-239.09 (0.29)	-239.60 (-0.22)	-239.39
H_2S	-175.90 (1.89)	-177.56 (0.23)	-177.41 (0.38)	-177.83 (-0.03)	-177.79
ME	3.22	0.95	0.12	-0.30	-
MAE	3.22	0.95	0.14	0.30	-

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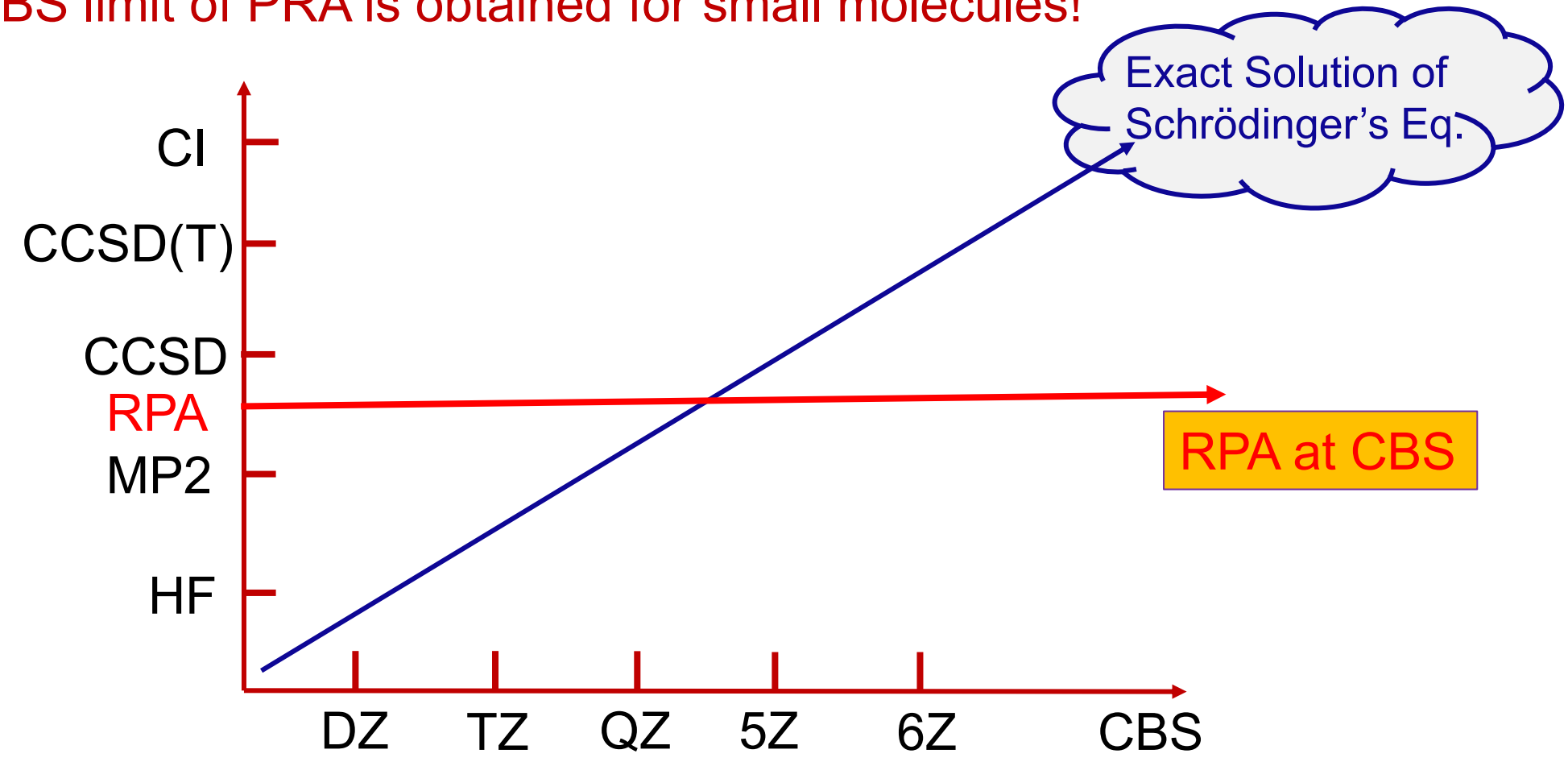
Summary

Genuine CBS limit of PRA is obtained for small molecules!



JCTC. **19**, 7199 (2023); PRA ***112***, *062819 (2025);* arXiv:2510.15570v2

Outlook

- Extending real-space *GW* to polyatomic molecules
- Extending to periodic systems
- Generating optimized correlation consistent NAO basis sets guided by the reference data

Acknowledgement

The work was mainly done by

Hao Peng（PhD student just graduated）

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  - Hong Jiang（Peking University）
  - Hongming Weng （Institute of Physics. CAS）
  - Haochen Liu & Hehu Xie （Institute of Mathematics, CAS）
  - Voker Blum (Duke University)

Thank you for your attention!