

Beyond LDA and GGA in practice

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DFT and beyond Hands-on tutorial workshop
Berlin, July 12-21, 2011

Beyond LDA and GGA in terms of many-body perturbation theory: theory and numerical practice

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- 1 Introduction of the “beyond-LDA/GGA approaches”
- 2 Implementation based on numeric atom-centered orbitals
- 3 Recent development of more accurate computational schemes
- 4 Conclusion

Density-functional theory to many-electron problems

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{ee}} = \sum_{i=1}^N \left[-\frac{1}{2} \nabla_i^2 + v_{\text{ext}}(\mathbf{r}_i) \right] + \sum_{i>j=1}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\hat{H}\Psi_k(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E_n \Psi_k(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

Kohn-Sham (KS) density-functional theory (DFT)

$$n(\mathbf{r}) = \langle \Psi_0 | \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i) | \Psi_0 \rangle = \sum_n^{\text{occ}} |\psi_n(\mathbf{r})|^2$$

$$E_0[n(\mathbf{r})] = T_s + E_{\text{ext}} + E_H + E_{\text{xc}}$$

$$E_{\text{ext}} = \int d\mathbf{r} v_{\text{ext}}(\mathbf{r}) n(\mathbf{r}); \quad E_H = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

$$T_s = \sum_n^{\text{occ}} \langle \psi_n | -\frac{1}{2} \nabla^2 | \psi_n \rangle$$

Exchange-correlation energy

$$E_{xc} = E_x + E_c$$

$$E_x = \langle \Phi_{KS} | V_{ee} | \Phi_{KS} \rangle - E_H$$

$$= -\frac{1}{2} \sum_{m,n}^{occ} \iint d\mathbf{r} d\mathbf{r}' \frac{\psi_n^*(\mathbf{r}) \psi_m(\mathbf{r}) \psi_m^*(\mathbf{r}') \psi_n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} := E_x^{EX}$$

$$E_c = \langle \Psi_0 | \hat{T} + \hat{V}_{ee} | \Psi_0 \rangle - \langle \Phi_{KS} | \hat{T} + \hat{V}_{ee} | \Phi_{KS} \rangle$$

$$= T_c + U_c$$

$$T_c = \langle \Psi_0 | \hat{T} | \Psi_0 \rangle - T_s; \quad U_c = \langle \Psi_0 | \hat{V}_{ee} | \Psi_0 \rangle - E_x^{EX}$$

- Explicitly density-dependent form for E_x must involve approximations
⇒ self-interaction error
- E_x and E_c are often approximated together
- If E_x is treated exactly, one must have a sophisticated (non-local) approximation to E_c to be compatible with E_x .

Practical approximations to E_{xc}

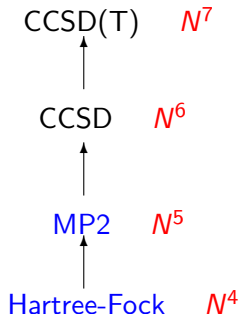
Jacob's ladder in DFT

RPA-type	unocc. $\psi_n(\mathbf{r})$	N^4-N^6
hybrids	occ. $\psi_n(\mathbf{r})$	N^4
meta-GGA	$\nabla^2 n(\mathbf{r})$	N^3
GGA	$\nabla n(\mathbf{r})$	N^3
LDA	$n(\mathbf{r})$	N^3

J. P. Perdew and K. Schmidt, in *Density Functional Theory and its Application to Materials*, (AIP, Melville, NY, 2001).

RPA: Random-phase approximation

Quantum chemistry approaches



MP2: second-order Möller-Plesset perturbation theory;

CCSD: Couple-cluster with singles and doubles

Shortcomings of explicit density-dependent functionals (LDA, GGAs, meta-GGAs):

- **Self-interaction error** \implies
 - too small band gaps in semi-conductors
 - underestimated chemical reaction barrier heights
 - failure to describe localized electrons in both solids and molecules
 - the exchange-correlation potential decays too fast for finite systems
 \implies unbound negative ions, no Rydberg states, etc.
- Unable to describe “strong correlations” (e.g., transition metal oxides)
- **Absence of van der Waals interactions** (true also for hybrid functionals)
- No access to electronic excited states

On the 4th rung of Jacob's ladder: hybrid functionals

$$E_{xc}^{\text{hyb}} = (1 - \alpha)E_x^{\text{GGA}} + \beta E_c^{\text{GGA}} + \alpha E_x^{\text{EX}}$$

Generalized Kohn-Sham (σ KS) single-particle equation

$\left[-\frac{1}{2} \nabla^2 + v_{\text{ext}}(\mathbf{r}) + v_{\text{xc}}(\mathbf{r}) \right] \psi(\mathbf{r}) = \epsilon \psi(\mathbf{r})$

Main features of hybrid functionals

- + Self-interaction is reduced, and the localized electronic states are treated much better.
- + The **generalized Kohn-Sham scheme** allows for obtaining a much better band gap, particularly for semiconductors.
- The van der Waals interactions are still absent
- The computational costs are dominated by the evaluation of the exact-exchange part.

$$0 < \beta < 1 \text{ (typically 1)}$$

D. Becke, J. Chem. Phys. 98, 1372 (1993); Seidl *et al.*, 53, 3764 (1996).

On the fifth rung of the Jacob's ladder

I. Adiabatic-connection fluctuation-dissipation theorem: a formally exact way for constructing E_{XC}

Imagine a continuum of fictitious systems governed by

$$\hat{H}_\lambda = \hat{T} + \hat{v}_{\text{ext}}^\lambda + \lambda \hat{V}_{\text{ee}} \quad (\text{where } 0 \leq \lambda \leq 1),$$

$$\hat{H}_\lambda |\Phi_\lambda[n]\rangle = E_\lambda |\Phi_\lambda[n]\rangle.$$

Exchange-correlation (XC) part of the interaction energy

$$U_{XC}^\lambda = \langle \Phi_\lambda[n] | V_{\text{ee}} | \Phi_\lambda[n] \rangle - \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Exact E_{XC} :
$$E_{XC} = \int_0^1 d\lambda U_{XC}^\lambda = U_{XC}^{\lambda=1} + T_c$$

D. C. Langreth and J. P. Perdew, Phys. Rev. B 15, 2884 (1977).

On the fifth rung of the Jacob's ladder: RPA

Fluctuation-Dissipation theorem

$$\underbrace{U_{XC}^\lambda}_{\text{Fluctuation}} = -\frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' v(\mathbf{r} - \mathbf{r}') \left[-\frac{1}{\pi} \int_0^\infty d\omega \underbrace{\text{Im} \chi_\lambda(\mathbf{r}, \mathbf{r}', \omega)}_{\text{Dissipation}} - n(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \right]$$

$\chi_\lambda(\mathbf{r}, \mathbf{r}', t - t') = \delta n(\mathbf{r}, t) / \delta v_{\text{ext}}^\lambda(\mathbf{r}', t')$: Response function
(the imaginary part describes the dissipation process)

$$\chi_\lambda = \chi_0 + \chi_0(\lambda v + f_{XC}^\lambda) \chi_\lambda \quad f_{XC} = \delta v_{XC} / \delta n$$

$$\chi_0(\mathbf{r}, \mathbf{r}', \omega) = 2 \sum_{mn} \frac{(f_n - f_m) \psi_m^*(\mathbf{r}) \psi_n(\mathbf{r}) \psi_n^*(\mathbf{r}') \psi_m(\mathbf{r}')}{\omega - \epsilon_m + \epsilon_n}$$

$0 \leq f_m \leq 1$: Fermi occupation number

$$\text{RPA} \iff f_{XC}^\lambda = 0$$

On the fifth rung of the Jacob's ladder: GL2/MP2

II. Many-body perturbation theory

$$\hat{H} = \hat{H}^0 + \hat{H}'$$

$$\hat{H}^0 = \sum_{i=1}^N \left[-\frac{1}{2} \nabla_i^2 + v^{\text{ext}}(\mathbf{r}) + v_i^{\text{MF}} \right]$$

$$\hat{H}' = \sum_{i < j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^N v_i^{\text{MF}}$$

$$\hat{H}^0 |\Phi_n\rangle = E_n^{(0)} |\Phi_n\rangle$$

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} + \dots$$

$$E_0^{(0)} = \langle \Phi_0 | \hat{H}^0 | \Phi_0 \rangle$$

$$E_0^{(1)} = \langle \Phi_0 | \hat{H}' | \Phi_0 \rangle$$

$$E_0^{(2)} = \sum_{n>0} \frac{|\langle \Phi_0 | H' | \Phi_n \rangle|^2}{E_0^{(0)} - E_n^{(0)}}$$

$v^{\text{MF}} = v^{\text{HF}}$ (HF potential) \implies Møller-Plesset perturbation theory

$v^{\text{MF}} = v^{\text{KS}}$ (KS potential) \implies Görling-Levy perturbation theory

A. Görling and M. Levy, Phys. Rev. B **47**, 13105 (1993).

S. Grimme, J. Chem. Phys. **122**, 034108 (2006). ([Double hybrids](#))

Diagrammatic (Goldstone) representation of cRPA

- Random phase approximation to the correlation energy

$$E_c^{RPA} = \text{[diagram 1]} + \text{[diagram 2]} + \dots$$

Advantages:

- The long-range vdW interactions are included.
- Compatible with exact-exchange, the inclusion of which cancels the self-interaction term present in the Hartree energy.

$$E_c^{MP2} = \text{[diagram 3]} + \text{[diagram 4]}$$

MP2: “second-order direct (ring) plus exchange terms”

Beyond LDA and GGA: hybrid functionals, GL2, RPA, and GW

Basic ingredients required:

- Full or a fraction of exact-exchange
 - **Exact-exchange** : the **first-order term** of the perturbation series based on the **Kohn-Sham** non-interacting reference Hamiltonian
- GL2 (MP2) or RPA-type correlation energy
 - **GL2 (MP2)** : the **second-order term** of the perturbation series based on the **Kohn-Sham (Hartree-Fock)** reference Hamiltonian
 - **RPA**: a partial summation of “ring” diagrams to infinite order
- **GW** self-energy (**talk by P. Rinke, Wed, Jul. 20**)
 - In analogy to **RPA**, but for the self-energy.

All can be formulated within the framework of many-body perturbation theory (either for total energy or the self-energy)

- 1 Introduction of the “beyond-LDA/GGA approaches”
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Beyond LDA and GGA in practice

Numeric atom-centered basis (NAO):

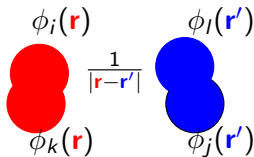
$$\phi_i(\mathbf{r}) = \frac{u_{nl}(r)}{r} Y_{lm}(\hat{\Omega})$$

- Well established for standard functionals (LDA and GGAs)
 - ▶ Flexible in shape \Rightarrow compactness
 - ▶ Natural inclusion of core electrons
 - ▶ Becoming more and more popular recently
Dmol, FPLO, FHI-aims, Siesta, etc.
- But how about doing exact-exchange and beyond (e.g., MP2, RPA et al.)?

Main challenges:

four-center Coulomb integrals

$$(ik|lj) = \int d\mathbf{r} d\mathbf{r}' \frac{\phi_i(\mathbf{r})\phi_k(\mathbf{r})\phi_l(\mathbf{r}')\phi_j(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$



Our solution: resolution of identity (RI), or “density fitting”

GW, RPA (noninteracting response function)

$$\chi(\mathbf{r}, \mathbf{r}', i\omega) = \sum_m^{\text{occ}} \sum_a^{\text{unocc}} \left[\psi_m(\mathbf{r})\psi_a(\mathbf{r})\psi_m(\mathbf{r}')\psi_a(\mathbf{r}') \frac{2(\varepsilon_m - \varepsilon_a)}{\omega^2 + (\varepsilon_m - \varepsilon_a)^2} \right]$$

Hartree-Fock (exchange matrix)

$$\Sigma_{ij}^x = \iint d\mathbf{r}d\mathbf{r}' \sum_n^{\text{occ}} \frac{\phi_i(\mathbf{r})\psi_n(\mathbf{r})\psi_n(\mathbf{r}')\phi_j(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

$$\psi_n(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})c_{in}$$

MP2 (Coulomb repulsion integral)

$$(ma|nb) = \iint d\mathbf{r}d\mathbf{r}' \frac{\psi_m(\mathbf{r})\psi_a(\mathbf{r})\psi_n(\mathbf{r}')\phi_b(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

“Density fitting”

$$\phi_i(\mathbf{r})\phi_j(\mathbf{r}) \approx \sum_{\mu} C_{ij}^{\mu} P_{\mu}(\mathbf{r})$$

$\phi_i(\mathbf{r})$: NAO basis; $\psi_n(\mathbf{r})$: single-particle KS/HF orbitals

RI with a set of auxiliary basis functions

- Observation: $N_{\text{basis}} \cdot (N_{\text{basis}} + 1)/2$ many pair products $\{\phi_i(\mathbf{r})\phi_j(\mathbf{r})\}$, where $i < j = 1, 2, \dots, N_{\text{basis}}$, are heavily linear dependent
- One can construct a linearly independent, auxiliary basis set $\{P_\mu(\mathbf{r})\}$, ($N_{\text{aux}} \sim N_{\text{basis}}$), sufficiently accurate to represent $\{\phi_i(\mathbf{r})\phi_j(\mathbf{r})\}$.

$$\phi_i(\mathbf{r})\phi_j(\mathbf{r}) \approx \sum_{\mu}^{N_{\text{aux}}} C_{ij}^{\mu} P_{\mu}(\mathbf{r})$$

- It follows (RI decomposition)

$$(ik|lj) \approx \sum_{\mu\nu} C_{ik}^{\mu} \langle P_{\mu}|v|P_{\nu} \rangle C_{lj}^{\nu} = \sum_{\mu\nu} C_{ik}^{\mu} V_{\mu\nu} C_{lj}^{\nu}$$

- Construct $\{P_{\mu}(\mathbf{r})\}$, and determine C_{ik}^{μ}

A simple

1. $\{P_\mu(\mathbf{r})\}$

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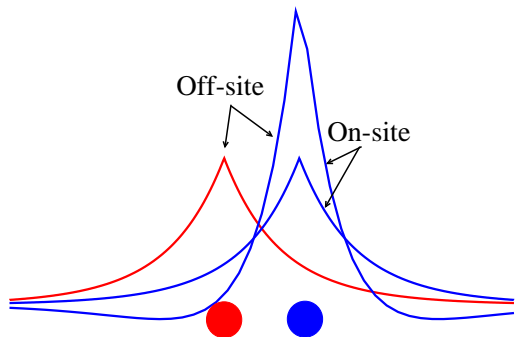
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3. Multi

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- "On-site" pairs $\phi_i(\mathbf{r} - \mathbf{R}_a)\phi_j(\mathbf{r} - \mathbf{R}_b)$ "exactly" represented by $P_\mu(\mathbf{r})$!
- But how about "off-site" pairs $\phi_i(\mathbf{r} - \mathbf{R}_b)\phi_j(\mathbf{r} - \mathbf{R}_a)$?

Determining C_{ik}^μ : “RI-SVS” vs “RI-V”

$$\phi_i(\mathbf{r})\phi_j(\mathbf{r}) \approx \sum_{\mu} C_{ij}^{\mu} P_{\mu}(\mathbf{r}); \quad \left(\delta\rho(\mathbf{r}) = \phi_i(\mathbf{r})\phi_k(\mathbf{r}) - \sum_{\mu} C_{ik}^{\mu} P_{\mu}(\mathbf{r}). \right)$$

minimizing $(\delta\rho|\delta\rho)$

minimizing $(\delta\rho|\delta\rho)$

$$C_{ik}^{\mu} = \sum_{\nu} (ik|\nu) S_{\nu\mu}^{-1}$$

$$(ik|\nu) = \int d\mathbf{r} \phi_i(\mathbf{r})\phi_k(\mathbf{r})P_{\nu}(\mathbf{r})$$

$$S_{\nu\mu} = \int d\mathbf{r} P_{\nu}(\mathbf{r})P_{\mu}(\mathbf{r})$$

$$(ik|lj) = \sum_{\mu\mu'\nu\nu'} (ik|\nu) S_{\nu\nu'}^{-1} V_{\nu'\mu'} V_{\mu'\mu}^{-1} (\mu|lj).$$

“RI-SVS” version

$$C_{ik}^{\mu} = \sum_{\nu} (ik|\nu) V_{\nu\mu}^{-1}$$

$$(ik|\nu) = \int d\mathbf{r} d\mathbf{r}' \phi_i(\mathbf{r})\phi_k(\mathbf{r})v(\mathbf{r}-\mathbf{r}')P_{\nu}(\mathbf{r}').$$

$$V_{\nu\mu} = \int d\mathbf{r} d\mathbf{r}' P_{\nu}(\mathbf{r})v(\mathbf{r}-\mathbf{r}')P_{\mu}(\mathbf{r}').$$

$$(ik|lj) = \sum_{\mu\nu} (ik|\nu) V_{\nu\mu}^{-1} (\mu|lj).$$

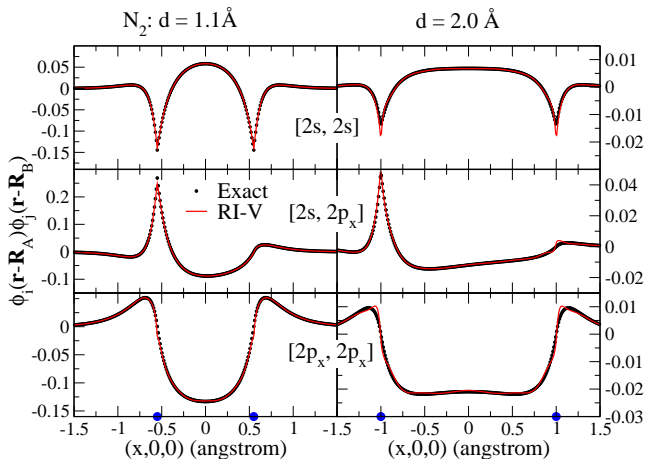
“RI-V” version

- “RI-V” gives much better accuracy
- A singular value decomposition ϵ^{svd} is introduced in the matrix inversion to prevent the possible illconditioning behavior.

Dunlap, Connolly, and Sabin, JCP **71**, 3396 (1979).

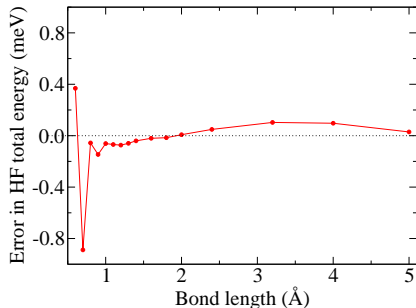
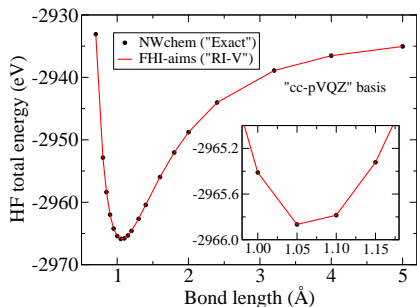
Vahtras, J. Almlöf, and Feyereisen, CPL **213**, 514 (1993).

On the accuracy of the RI approximation (for off-site pairs)



- NAO *tier 2* basis set (4s3p2d1f1g) is used in the auxiliary basis construction

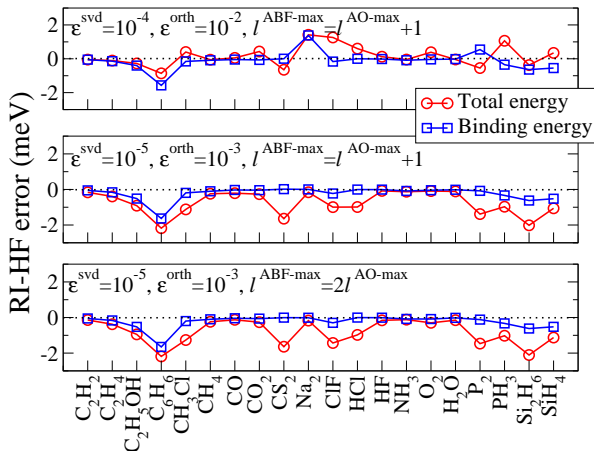
Accuracy of the RI approximation: HF total energy for N₂



- Gaussian basis set "cc-pVQZ" is used.
- Reference values are obtained with NWchem.
- Thresholding parameters

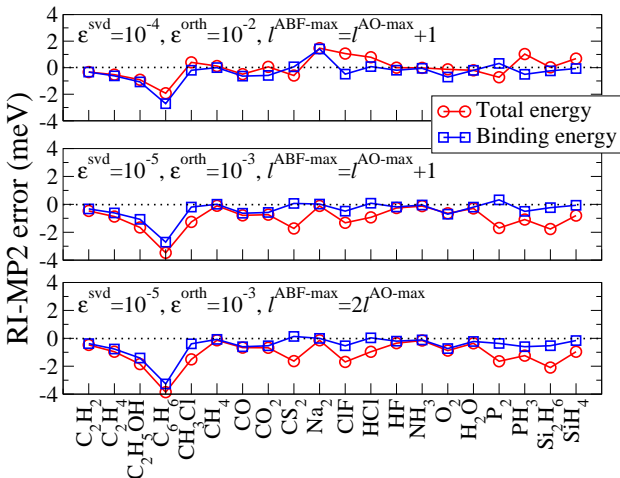
$$J^{ABF-max} = J^{AO-max} + 1, \epsilon^{orth} = 10^{-2}, \epsilon^{svd} = 10^{-4}$$

On the accuracy of RI-HF for light elements



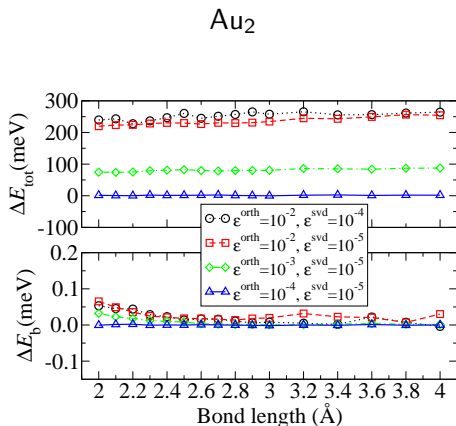
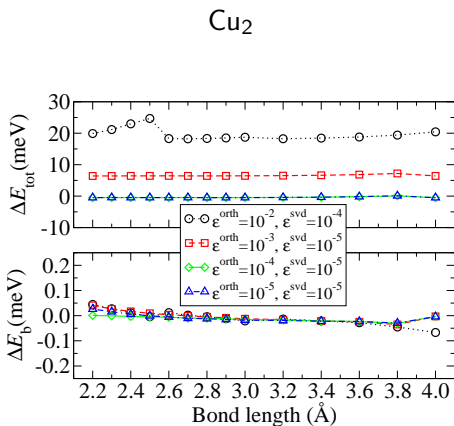
- Gaussian cc-pVQZ basis set is used
- “RI-free” NWchem results are used as reference

On the accuracy of RI-MP2 for light elements



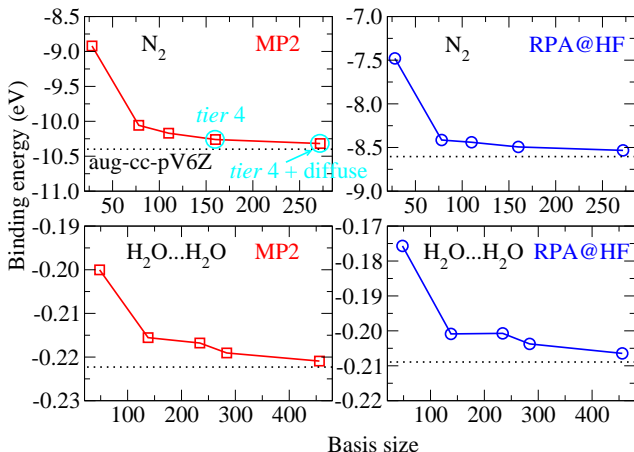
- Gaussian cc-pVQZ basis set is used
- “RI-free” NWchem results are used as reference

On the accuracy of RI-HF for heavy elements



Tighter ϵ^{orth} parameter is needed for heavy elements, but meV/atom total-energy accuracy can still be achieved with $\epsilon^{\text{orth}} = 10^{-4}$ and tighter.

Convergence with NAO basis sets



NAOs for N:

tier 1: $3s2p1d$

tier 2: $4s3p2d1f1g$

tier 3: $5s4p3d2f1g$

tier 4: $6s5p4d3f2g$

(80)

diffuse functions from
aug-cc-pV5Z

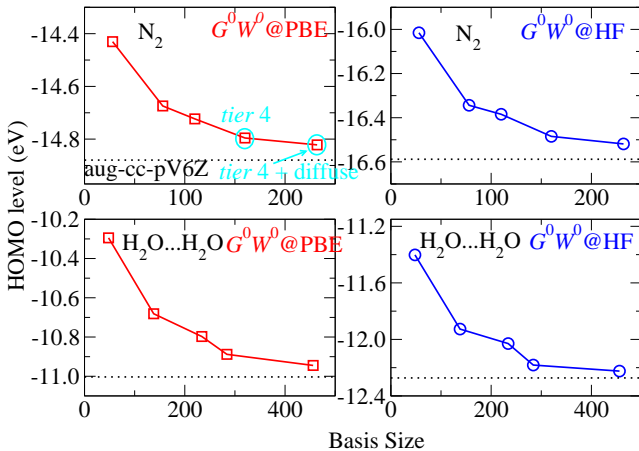
$1s1p1d1f1g1h$ (36)

aug-cc-pV6Z:

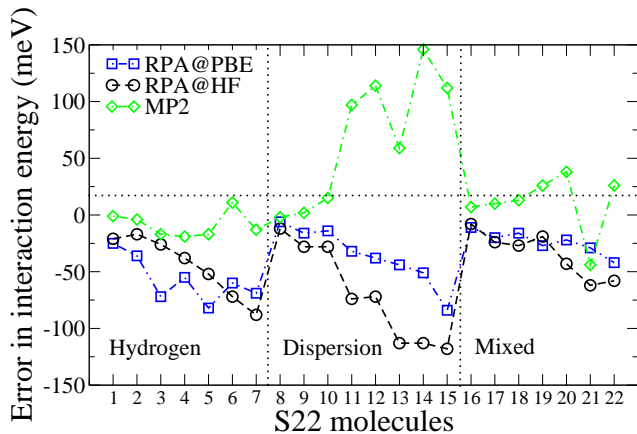
$8s7p6d5f4g3h2i$

(189)

Convergence with NAO basis sets



Application I: Binding energies for molecules



S22 molecular set:

Jurečka *et al.*, PCCP 8,1985 (2006)

- 7 hydrogen-bonded molecules
- 8 dispersion bonded molecules
- 7 with mixed character

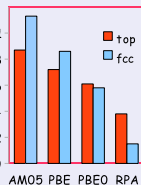
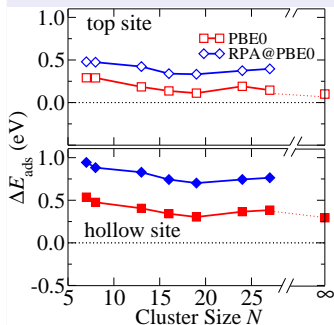
Application II: Adsorption problem

Delta-XC correction scheme

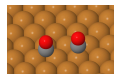
$$E_{\text{ads}}(\text{XC-better}) = E_{\text{ads}}(\text{PBE}) + \lim_{\text{cluster} \rightarrow \infty} [E_{\text{ads}}^{\text{cluster}}(\text{XC-better}) - E_{\text{ads}}^{\text{cluster}}(\text{PBE})]$$

Hu, Reuter, and Scheffler, PRL **98**, 176103 (2007).

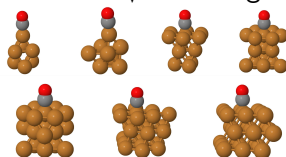
PBE0 and RPA calculation for CO@Cu(111)



Ren, Rinke, and Scheffler, PRB, **80**, 045402 (2009).



Cluster \downarrow modeling

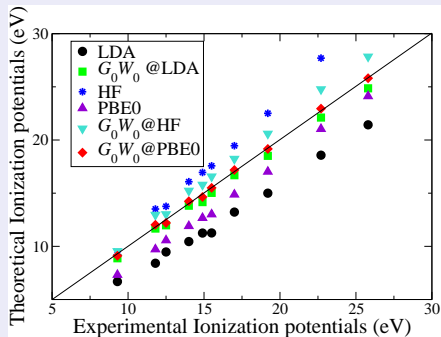


Application III: G^0W^0 quasiparticle energy corrections

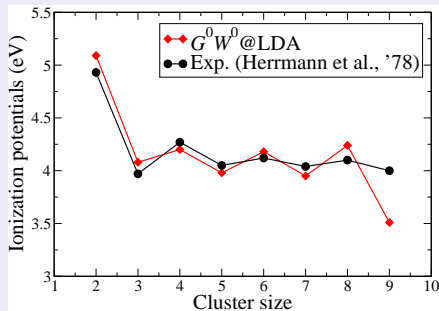
G^0W^0 correction to KS energy levels

$$E_n^{G^0W^0} = E_n^{KS} + \sum_{nn}^{G^0W^0} (E_n^{G^0W^0}) - V_n^{xc}$$

Ionization potentials for benzene



Ionization potentials for Na clusters



- 1 Introduction of the “beyond-LDA/GGA approaches”
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Exact-exchange plus the correlation energy in the random phase approximation (EX+cRPA)

⇒ A promising route to go beyond (semi-)local DFT

- Self-interaction in (semi-)local DFT is reduced in EX+cRPA; (cRPA is not self-correlation free though)
 - Correct asymptotic Kohn-Sham potential for finite systems
- cRPA is fully non-local, and van der Waals interactions are included automatically;
- Applicable to molecules, insulators, and metals with various bonding natures. (In contrast to second-order perturbation theory like MP2)

RPA calculations in practice

In practical calculations, RPA is done perturbatively on a LDA/GGA reference (e.g., RPA@PBE)

The “standard” RPA scheme:

$$\begin{aligned} E^{\text{RPA@PBE}} &= E^{\text{PBE}} - E_{\text{xc}}^{\text{PBE}} + \left(E_{\text{x}}^{\text{exact}} + E_{\text{c}}^{\text{RPA}} \right) @\text{PBE} \\ &= \left(E_{\text{kin}} + E_{\text{ext}} + E_{\text{Hartree}} + E_{\text{x}}^{\text{exact}} + E_{\text{c}}^{\text{RPA}} \right) @\text{PBE} \\ &= E^{\text{EX@PBE}} + E^{\text{cRPA@PBE}} \end{aligned}$$

$E^{\text{EX@PBE}}$: non-self-consistent Hartree-Fock energy (exchange-only total energy) evaluated with PBE orbitals.

$E^{\text{cRPA@PBE}}$: RPA correlation energy evaluated with PBE orbitals.

But, the “standard” RPA scheme underestimates the bond strength systematically

Rayleigh-Schrödinger perturbation theory

Perturbative correction to the ground state energy:

Hartree-Fock vs Kohn-Sham reference

$$H^{(0)} = H^{\text{HF}}; |\Phi_0\rangle = |\Phi_{\text{HF}}\rangle$$

$$E_0^{(0)} + E_0^{(1)} = E^{\text{HF}}$$

$$E_c^{\text{SE}} = 0 \text{ (Brillouin theorem)}$$

$$H^{(0)} = H^{\text{PBE}}; |\Phi_0\rangle = |\Phi_{\text{PBE}}\rangle$$

$$E_0^{(0)} + E_0^{(1)} = E^{\text{EX@PBE}}$$

$$E_c^{\text{SE}} = \sum_{ia} \frac{|\langle a | \hat{v}_{\text{HF}} - \hat{v}_{\text{KS-PBE}} | i \rangle|^2}{\epsilon_i - \epsilon_a} \neq 0$$

(but not included in the RPA@PBE)

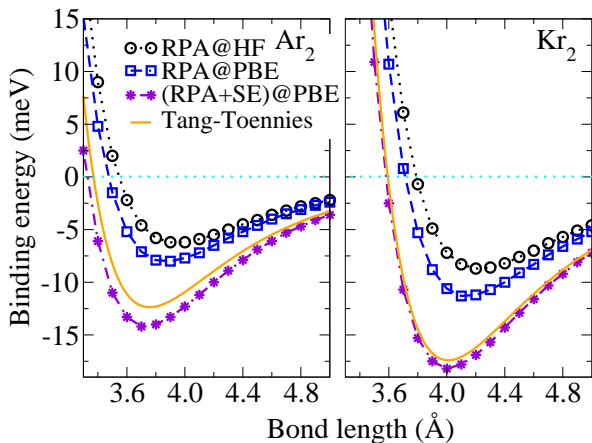
Kohn-Sham many-body perturbation theory

A. Görling and M. Levy, Phys. Rev. B **47**, 13105 (1993);

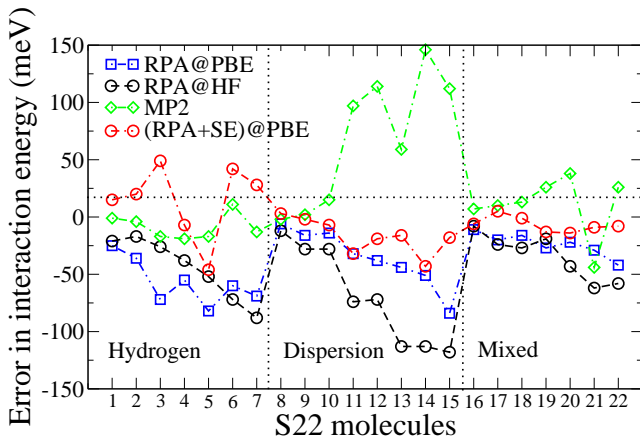
H. Jiang and E. Engel, J. Chem. Phys. **125**, 184108 (2006).

$$E_c^{\text{RPA+SE}} = E_c^{\text{RPA}} + E_c^{\text{SE}}$$

Performance of the RPA+SE for Ar₂ and Kr₂



Performance of the RPA+SE for S22



MAE: 18 meV

X. Ren, A. Tkatchenko, P. Rinke, and M. Scheffler, Phys. Rev. Lett. 106, 153003 (2011).

- 1 Introduction of the “beyond-LDA/GGA approaches”
- 2 Implementation based on numeric atom-centered orbitals
- 3 Recent development of more accurate computational schemes
- 4 Conclusion

Conclusions

- The RI technique makes the NAO basis functions a competitive option for the implementation of approaches beyond LDA and GGA.
 - ▶ hybrid functionals
 - ▶ MP2
 - ▶ RPA and *GW*
- can treat system size ~ 100 light atoms \dots .
- The many-body perturbation theory offers a useful perspective for designing more elaborate functionals in the higher rungs of Jacob's ladder.

On-going work

- Periodic extension (Sergey Levchenko, Jürgen Wieferink)
- Fully self-consistent *GW* (Fabio Caruso)

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Code development

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Method development

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Matthias Scheffler

Thank you!