

Excitation energy calculations with (nearly) exact Kohn-Sham potentials

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occupied orbital energies

LDA/GGA: typically 4 – 6 eV too high
(HF typically 1 eV too low)

An error of 100 – 140 kcal/mol, totally unacceptable
in the total energy

HF, DFA and exact KS HOMO orbital energies

	HF	LDA	BLYP	$-IP = \epsilon_{KS}$
H ₂	-16.18	-10.26	-10.39	-16.44
H ₂ O	-13.88	-7.40	-7.21	-12.62
HF	-17.69	-9.82	-9.64	-16.19
N ₂	-16.71	-11.89	-11.49	-16.68
CO	-15.1	-9.11	-9.00	-14.01
HCN	-13.50	-9.23	-8.87	-13.61
FCN	-13.65	-8.97	-8.62	-13.67
HCl	-12.98	-8.15	-7.91	-12.77

KS HOMO is equal to $-I$;

HF HOMO is appr. equal to $-I$ (frozen orbital approx.)

LDA, GGA orbital energies are upshifted by ca. 4 - 6 eV
(uniformly: occup. and unoccup *valence* orbitals)

occupied orbital energies

- LDA/GGA: typically 4 – 6 eV too high
(HF typically 1 eV too low)

Why?

- Not because of wrong asymptotics of potentials
- Not because of self-interaction error

But because LDA/GGA potentials are strongly upshifted in the bulk molecular region for a different reason

orbital energy determined by bulk molecular region

$$\varepsilon_i = \left\langle \psi_i(\mathbf{r}) \left| -\frac{1}{2} \nabla^2 + V_{nuc}(\mathbf{r}) + V_{Coul}(\mathbf{r}) + V_{XC}(\mathbf{r}) \right| \psi_i(\mathbf{r}) \right\rangle$$

Determined by molecular region where $\psi_i(\mathbf{r})$ has largest amplitude and where potentials

$V_{nuc}(\mathbf{r})$, $V_{Coul}(\mathbf{r})$, $V_{XC}(\mathbf{r})$ are large.

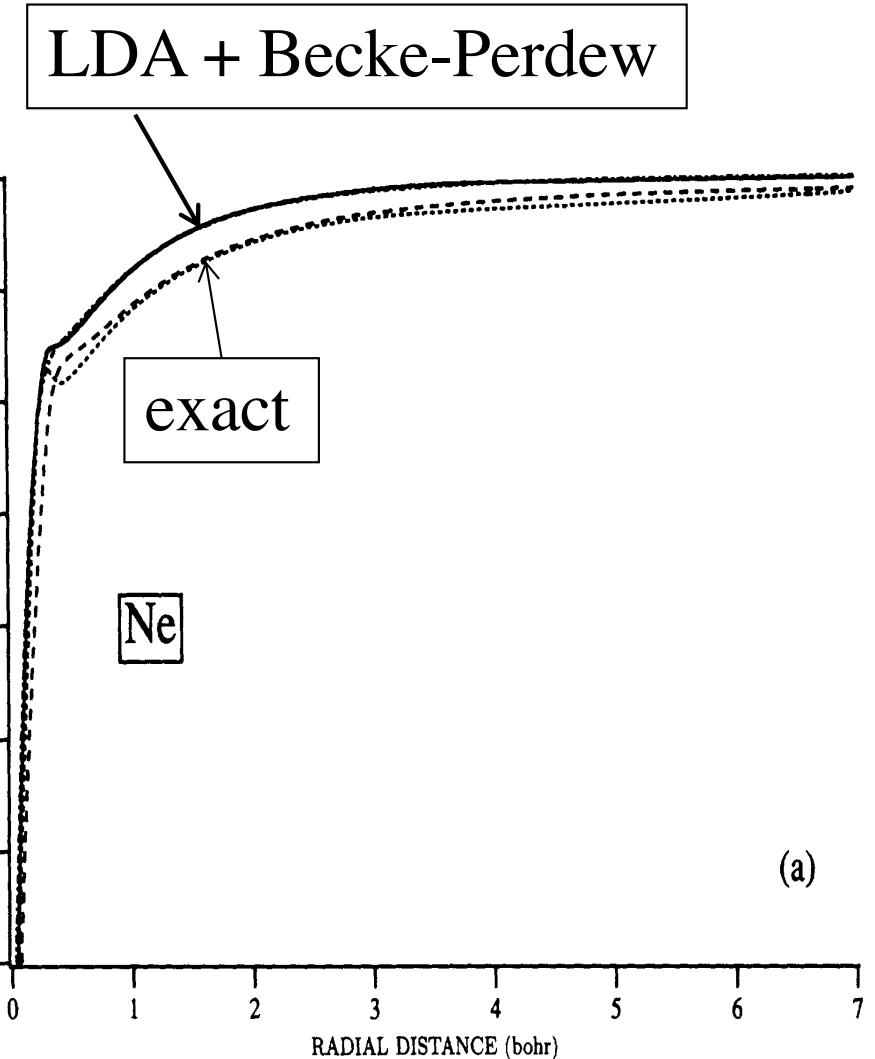
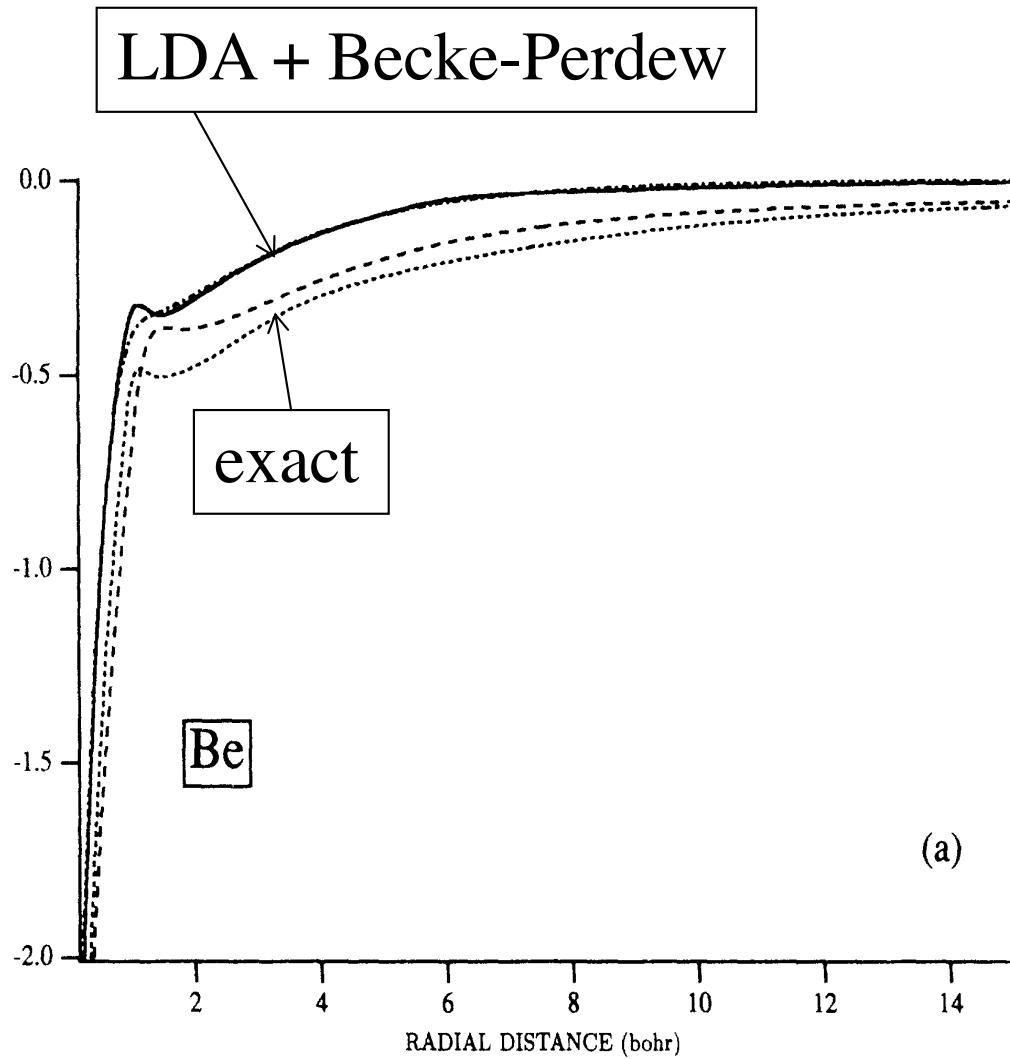
Asymptotic regions contribute little!

(Except for Rydberg orbitals.)

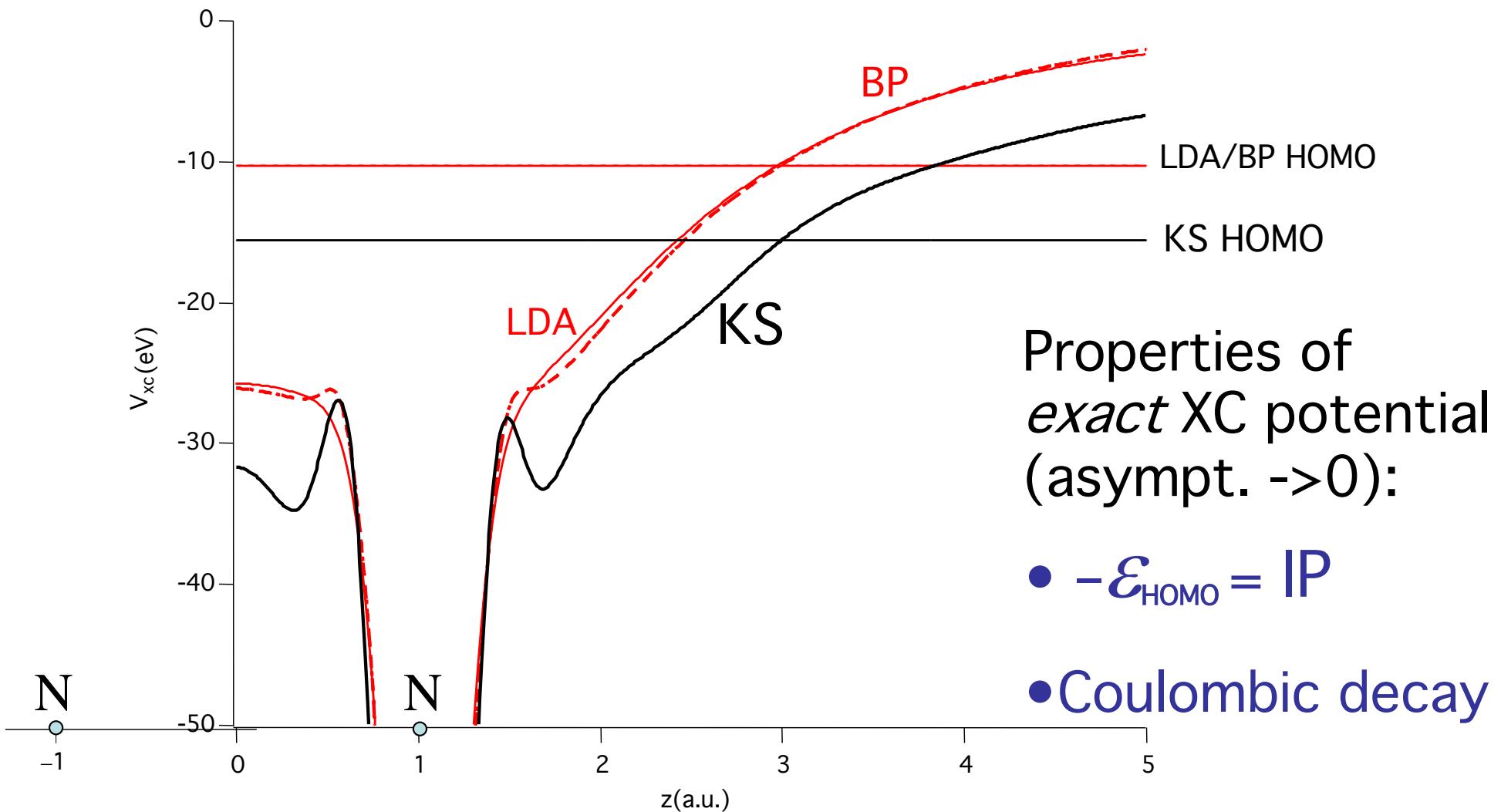
Too high orbital energies:

*LDA/GGA potentials are strongly upshifted
in the bulk molecular region*

Exact and LDA KS potentials

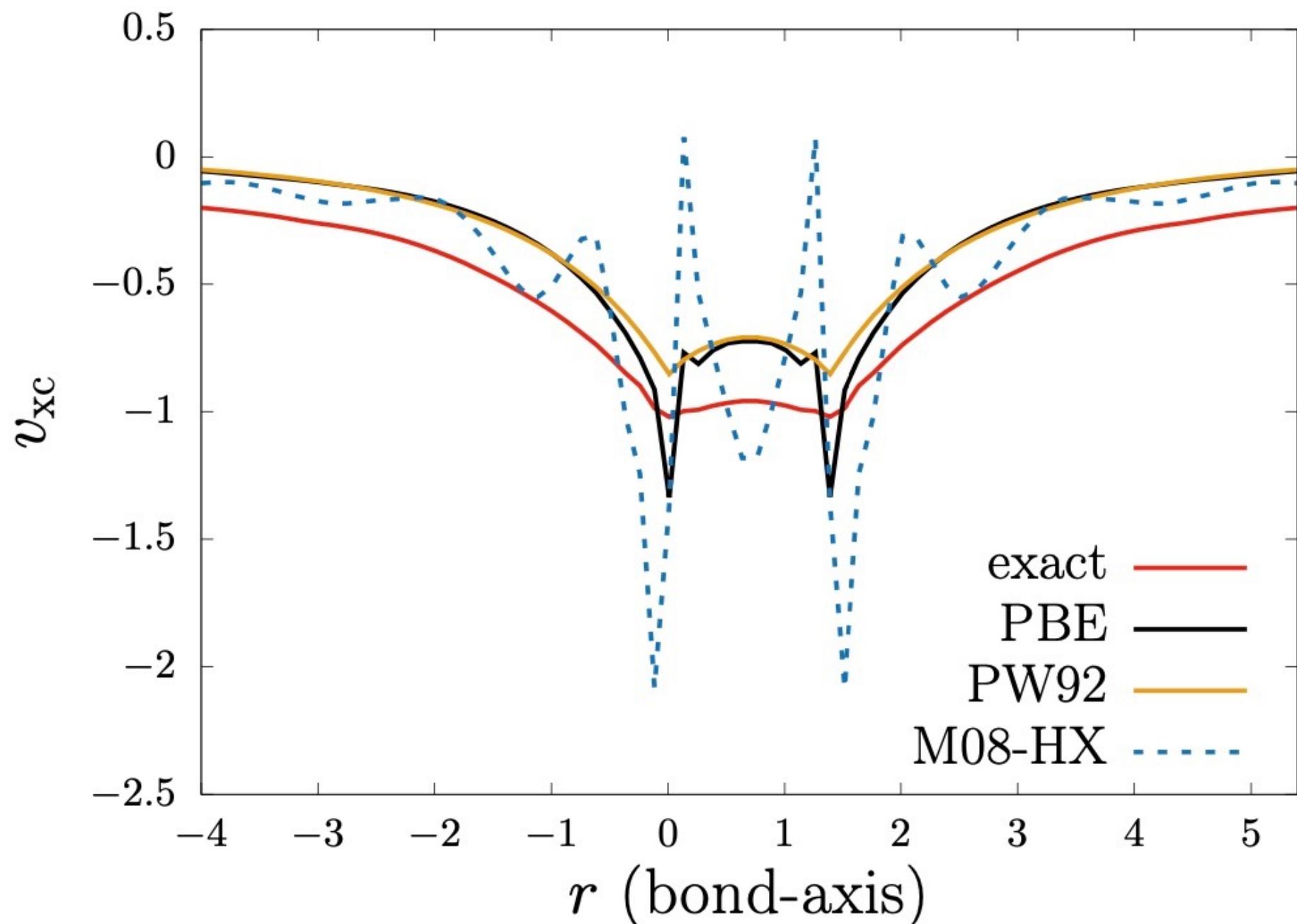


N_2 : XC potentials along bond axis

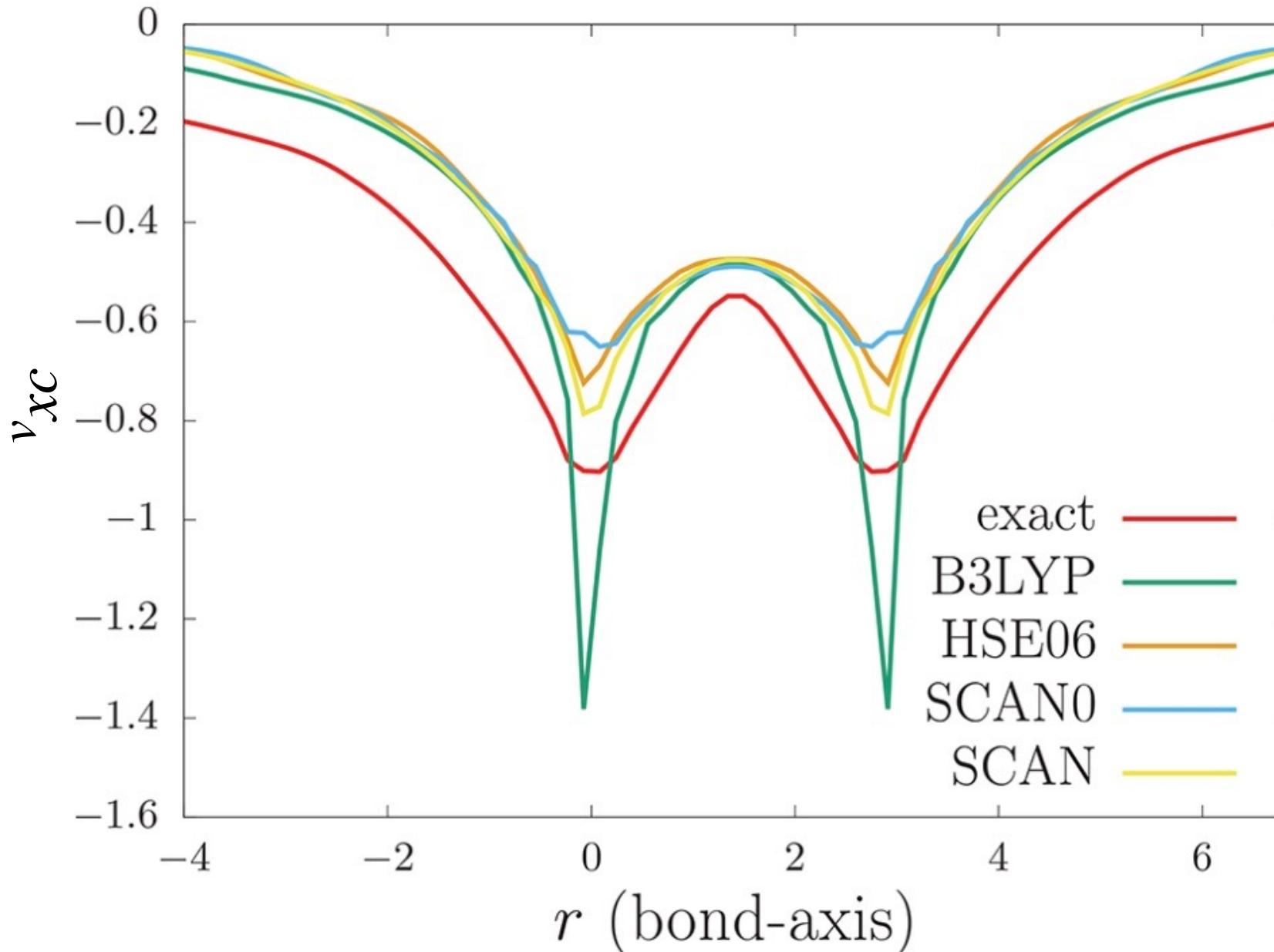


Grüning, Gritsenko, Baerends, JCP 2002

Gavini et al. JPCL 12(2021): H₂ at R_e



Gavini et al. JPCL 12(2021): H₂ at 2R_e



Why is LDA/GGA potential so upshifted?
Because response part of potential is wrong!

$$E_{XC} \equiv \int \rho(\mathbf{r}) \varepsilon_{XC}(\mathbf{r}) d\mathbf{r}$$

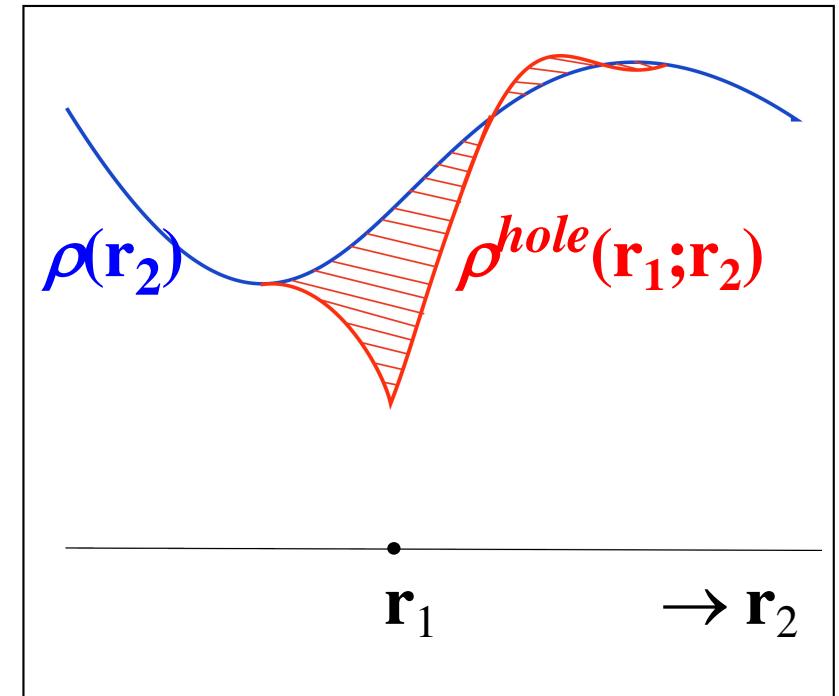
$$= \frac{1}{2} \int \rho(\mathbf{r}) \bar{v}_{XC}^{hole}(\mathbf{r}) d\mathbf{r}$$

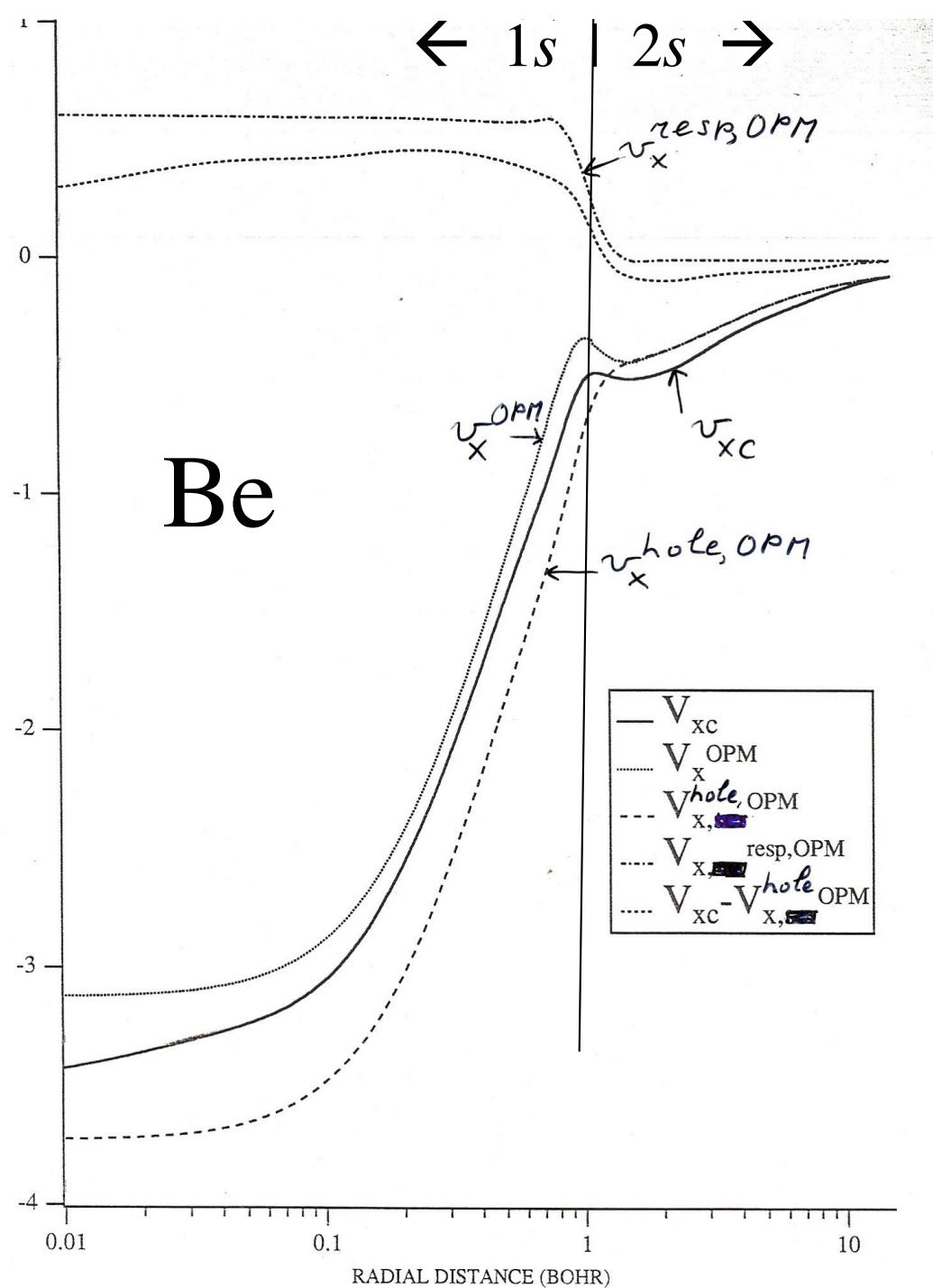
$$\Rightarrow \varepsilon_{XC}(\mathbf{r}) = \frac{1}{2} \bar{v}_{XC}^{hole}(\mathbf{r}_1)$$

$$v_{XC}(\mathbf{r}) = \frac{\delta E_{XC}}{\delta \rho(\mathbf{r})} = \varepsilon_{XC}(\mathbf{r}) + \int \rho(\mathbf{r}_1) \frac{\delta \varepsilon_{XC}(\mathbf{r}_1)}{\delta \rho(\mathbf{r})} d\mathbf{r}_1$$



$$\frac{1}{2} \bar{v}_{XC}^{hole}(\mathbf{r}) + \frac{1}{2} \bar{v}_{XC}^{hole}(\mathbf{r}) + v_{XC}^{resp}(\mathbf{r})$$

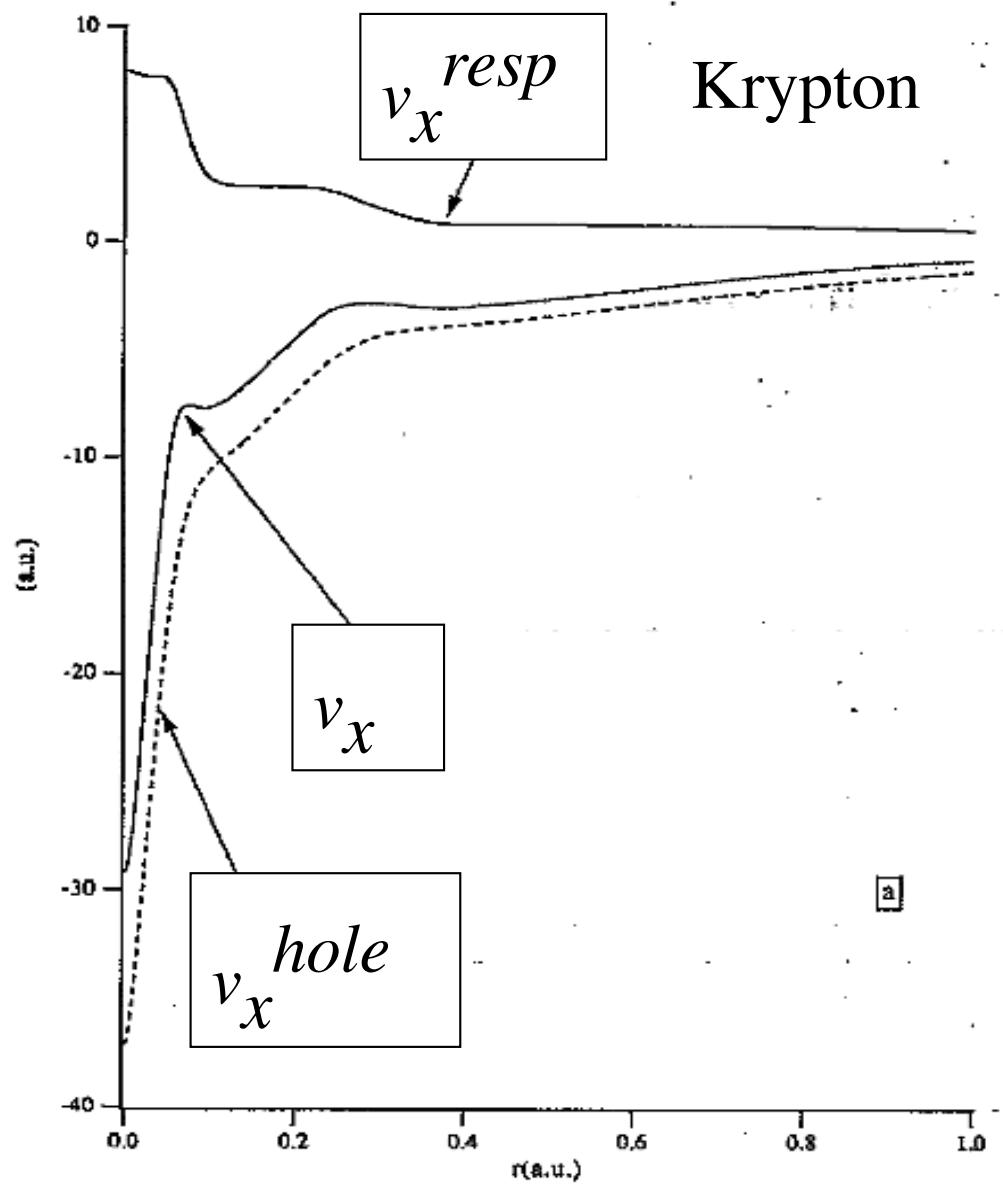




How does response potential look?

It has steps;
zero in HOMO
region

Steps in the (exchange) pot. of Krypton come from
response part of pot.



O. Gritsenko, R. van Leeuwen,
E. J. Baerends
J. Chem. Phys. **101** (1994) 8955

exact expression for v^{resp} : $v^{N-1} - v_s^{N-1}$

$$v^{resp}(1) = v^{N-1}(1) - v_s^{N-1}(1) = \sum_j \frac{|d_j(1)|^2}{\rho(1)} (I_j - I_0) - \sum_j \frac{|\psi_j^s(1)|^2}{\rho(1)} (-\varepsilon_j - I_0)$$

Dyson orbitals:
very similar to KS orbitals
and HF orbitals for
primary ion states

exact ionization energies

The response potential consists of contributions that have step like behavior when going from one shell to the next in an atom or molecule

LDA/GGA response pot.: no steps!

$$E_X^{LDA} = \int \rho(\mathbf{r}) \varepsilon_X^{LDA}(\mathbf{r}) d\mathbf{r} = \frac{1}{2} \int \rho(\mathbf{r}) v_{Xhole}^{EG}(\mathbf{r}) d\mathbf{r}$$

$$v_{Xhole}^{EG}(\mathbf{r}) = -3 \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}}$$

Long before LDA:

Slater: square hole around position \mathbf{r} of electron with depth $-(1/2)\rho(\mathbf{r})$,
integrating to -1 , gives practically same potential $C\rho(\mathbf{r})^{1/3}$

Slater (band structure theorists) applied this in one-electron equations
as exchange potential

Gaspar-Kohn-Sham (DFT):

Proper variational derivation of one-el. equations for the optimal orbitals yields:

$$\nu_X^{LDA}(\mathbf{r}) = \frac{2}{3} \nu_{Xhole}^{EG}(\mathbf{r})$$

→ Slater's X α method: use potential $\alpha \cdot \nu_{Xhole}^{EG}(\mathbf{r})$

α has been determined in various ways in atoms (e.g. K. Schwarz, 1972):

- exact exchange energy optimized;
- Virial Theorem obeyed
- energy equal to Hartree-Fock energy

→ α in range 0.78 (lightest elements) – 0.71 (beyond first row)

or in molecules (E. J. Baerends, 1973) ($\alpha = 0.70$)

→Slater's X α method: use potential αv_{Xhole}^{EG}

Actually, Slater resisted initially:

- orbital energies are “better” with full Slater (EG) exchange pot.!

J.C. Slater, *Quantum Theory of Molecules and Solids*,
Vol. 3 (1967): *Insulators, semiconductors and metals*

p. 243: Some writers have felt that on account of the importance of the variation principle for the total energy, it was more important to use ...
an exchange correction determined by variation of the total energy ...

The author does not agree with this point of view, feeling that the one-electron energies are more important in energy-band calculations.

The slightly different wavefunctions which we find by use of [the full $v_{Xhole}^{EG}(\mathbf{r})$] rather than $(2/3)v_{Xhole}^{EG}(\mathbf{r})$ will only make a second order change in the total energy.

Orbital energies from Slater (EG), LDA/GGA compared to exact KS

\mathbf{N}_2	$3\sigma_g$	$1\pi_u$	$2\sigma_u$
$-I_i$	- 15.58	- 16.83	- 18.75
ϵ_i (KS)	- 15.58	- 16.84	- 18.89
ϵ_i (Slater)	- 15.39	- 16.66	- 18.62
ϵ_i (BLYP)	- 10.28	- 11.49	- 13.39

Gritsenko, Mentel, Baerends, JCP 144 (2016) 204114

Orbital energies from Slater (EG), LDA, GGA compared to exact KS

H₂CO	2b₂	1b₁	5a₁	1b₂	4a₁
$-I_i$	- 10.9	- 14.5	- 16.1	- 17.0	- 21.4
ϵ_i (KS)	- 10.90	- 14.26	- 15.51	- 16.46	- 20.04
ϵ_i (Slater)	- 10.99	- 14.56	- 15.91	- 16.82	- 20.57
ϵ_i (BLYP)	- 6.22	- 9.94	- 10.93	- 12.08	- 15.59

Gritsenko, Mentel, Baerends, JCP 144 (2016) 204114

The LDA X-response pot. is (way) too repulsive

$$v_X^{LDA}(\mathbf{r}) = \frac{2}{3} v_{Xhole}^{EG}(\mathbf{r}) = -\frac{2}{3} 3 \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}} = -2 \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}}$$

$$v_X^{LDA}(\mathbf{r}) = -2 \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}} = -3 \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}} + \left(\frac{3}{8\pi} \right)^{\frac{1}{3}} \rho(\mathbf{r})^{\frac{1}{3}}$$
$$v_{Xhole}^{EG}(\mathbf{r}) \quad + v_{Xresp}^{LDA}(\mathbf{r})$$

(1 / 3) of hole pot.!
(1 / 2) of total X pot.!

*Wrong response potential causes
uniform upshift of orbital energies!*

How to model the response potential?

Krieger-Li-Iafrate (1994) derived a good approximation to the OEP potential in the exact-exchange only case:

$$\nu_X^{KLI}(\mathbf{r}) \approx \nu_{X\text{hole}}^{HF} + \sum_{i=1}^H w_i \frac{|\psi_i(\mathbf{r})|^2}{\rho(\mathbf{r})}$$

KLI exch.-response pot.: steps of height w_i

Approximation (GLLB) of v_{Xresp}

Step behavior introduced with $w_i = f(\varepsilon_F - \varepsilon_i)$

scaling density $\rho_\lambda(\mathbf{r}) = \lambda^3 \rho(\lambda \mathbf{r})$ yields $v_x[\rho_\lambda](\mathbf{r}) = \lambda v_x[\rho](\lambda \mathbf{r})$

dictates, with $\varepsilon_i[\rho_\lambda] = \lambda^2 \varepsilon_i[\rho]$,

$f(\lambda^2(\varepsilon_F - \varepsilon_i)) = \lambda f(\varepsilon_F - \varepsilon_i)$ so f must be prop. to square root:

$$f \rightarrow K \sqrt{\varepsilon_F - \varepsilon_i}$$

$$v_{Xresp}^{GLLB}(\mathbf{r}) = K[\rho] \sum_{i=1}^H \sqrt{\varepsilon_F - \varepsilon_i} \frac{|\psi_i(\mathbf{r})|^2}{\rho(\mathbf{r})} \quad \text{Exact in EG with } K = 0.382$$

Gritsenko, van Leeuwen, van Lenthe, Baerends, PRA 1995

Build up correct potential:

- 1) $v_X^{hole}(\mathbf{r})$ from $2\epsilon_X^{GGA}[\rho(\mathbf{r})](\mathbf{r}) = 2\epsilon_X^{LDA}(\mathbf{r}) + 2\epsilon_X^{B88}(\mathbf{r})$
 - $2\epsilon_X^{LDA}(\mathbf{r}) = v_{Xhole}^{LDA}(\mathbf{r})$ no factor 2/3!
 - note: B88 correction makes energy density go like $-1/2r$
so $v_{Xhole}^{B88}(\mathbf{r})$ has proper $-1/r$ asymptotics
- 2) $v_X^{resp}(\mathbf{r})$ taken as $v_{Xresp}^{GLLB}(\mathbf{r})$
- 3) correlation potential (hole + resp.) from LDA: $v_{corr}^{VWN}(\mathbf{r})$

---> B-GLLB-VWN

N₂ orbital energies

N ₂ (K=0.382)	3σ _g (HOMO)	2π _u	2σ _u	2σ _g
$\nu_{xhole,ii}$ (LDA)	- 24.89	- 23.51	- 24.72	- 29.47
$\nu_{xhole,ii}$ (B)	- 2.54	- 2.48	- 2.52	- 1.83
$\nu_{xresp,ii}$ (GLLB)	+ 4.56	+ 5.10	+ 3.97	+ 6.05
$\nu_{c,ii}$ (VWN)	- 1.76	- 1.75	- 1.76	- 1.91
$\nu_{xctot,ii}$	- 24.63	- 22.63	- 25.03	- 27.16
$h_{ii} + \nu_{H,ii}$	+ 8.89	+ 6.16	+ 5.73	- 6.17
ε_i (BGLLBVWN)	- 15.74	- 16.47	- 19.30	- 33.33
ε_i (KS)	- 15.58	- 16.84	- 18.89	- 33.67
$\Delta\varepsilon_i$	- 0.16	0.37	- 0.41	0.34

N₂ orbital energies

N ₂ (K=0.382)	$3\sigma_g$ (HOMO)	$2\pi_u$	$2\sigma_u$	$2\sigma_g$
$\nu_{xhole,ii}$ (LDA)	- 24.89	- 23.51	- 24.72	- 29.47
$\nu_{xhole,ii}$ (B)	- 2.54	- 2.48	- 2.52	- 1.83
$\nu_{xresp,ii}$ (GLLB)	+ 4.56	+ 5.10	+ 3.97	+ 6.05
$\nu_{c,ii}$ (VWN)	- 1.76	- 1.75	- 1.76	- 1.91
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$h_{ii} + \nu_{H,ii}$	+ 8.89	+ 6.16	+ 5.73	- 6.17
ε_i (BGLLBVWN)	- 15.74	- 16.47	- 19.30	- 33.33
ε_i (KS)	- 15.58	- 16.84	- 18.89	- 33.67
$\Delta\varepsilon_i$	- 0.16	0.37	- 0.41	0.34
$\Delta\varepsilon_i$ (LDA+B-KS)	4.82	4.91	4.99	5.00

HCOOH orbital energies (K=0.34)

	10a' HOMO	2a''	9a'	1a''	8a'	7a'
$v_{xhole,ii}$ (LDA)	-27.33	-27.95	-27.16	-25.03	-28.02	-24.38
$v_{xhole,ii}$ (B)	-2.63	-2.63	-2.57	-2.55	-2.61	-2.32
$v_{xresp,ii}$ (GLLB)	+4.86	+5.64	+5.74	+5.86	+5.69	+5.64
$v_{c,ii}$ (VWN)	-1.83	-1.85	-1.83	-1.78	-1.87	-1.78
$v_{xctot,ii}$	-26.94	-26.81	-25.82	-23.50	-26.79	-22.83
$h_{ii} + v_{H,ii}$	+15.33	+14.20	+11.59	+8.06	+10.20	+5.68
ε_i (BGLLBVWN)	-11.61	-12.61	-14.23	-15.44	-16.59	-17.15
ε_i (KS)	-11.51	-12.38	-14.48	-15.43	-16.64	-17.27
$\Delta\varepsilon_i$	-0.10	-0.23	0.25	-0.01	0.05	0.12
$\Delta\varepsilon_i$ (LDA+B)	4.23	3.82	4.07	3.78	4.17	3.82

HCOOH lower orbital energies (K=0.34)

	7a'	6a'	5a'	4a'
$\nu_{xhole,ii}$ (LDA)	- 24.38	- 24.95	- 31.36	- 29.60
$\nu_{xhole,ii}$ (B)	- 2.32	- 2.24	- 2.08	- 2.05
$\nu_{xresp,ii}$ (GLLB)	+ 5.64	+ 5.99	+ 5.91	+ 6.12
$\nu_{c,ii}$ (VWN)	- 1.78	- 1.79	- 1.95	- 1.90
$\nu_{xctot,ii}$	- 22.83	- 23.01	- 29.48	- 27.44
$h_{ii} + \nu_{H,ii}$	+ 5.68	+ 2.17	- 1.11	- 5.41
ε_i (BGLLBVWN)	- 17.15	- 20.84	- 30.95	- 32.85
ε_i (KS)	- 17.27	- 21.17	- 30.43	- 32.94
$\Delta\varepsilon_i$	0.12	- 0.33	- 0.16	0.09
$\Delta\varepsilon_i$ (LDA+B-KS)	3.82	3.88	4.14	4.14

Good orbital energies (not upshifted) very important in anions

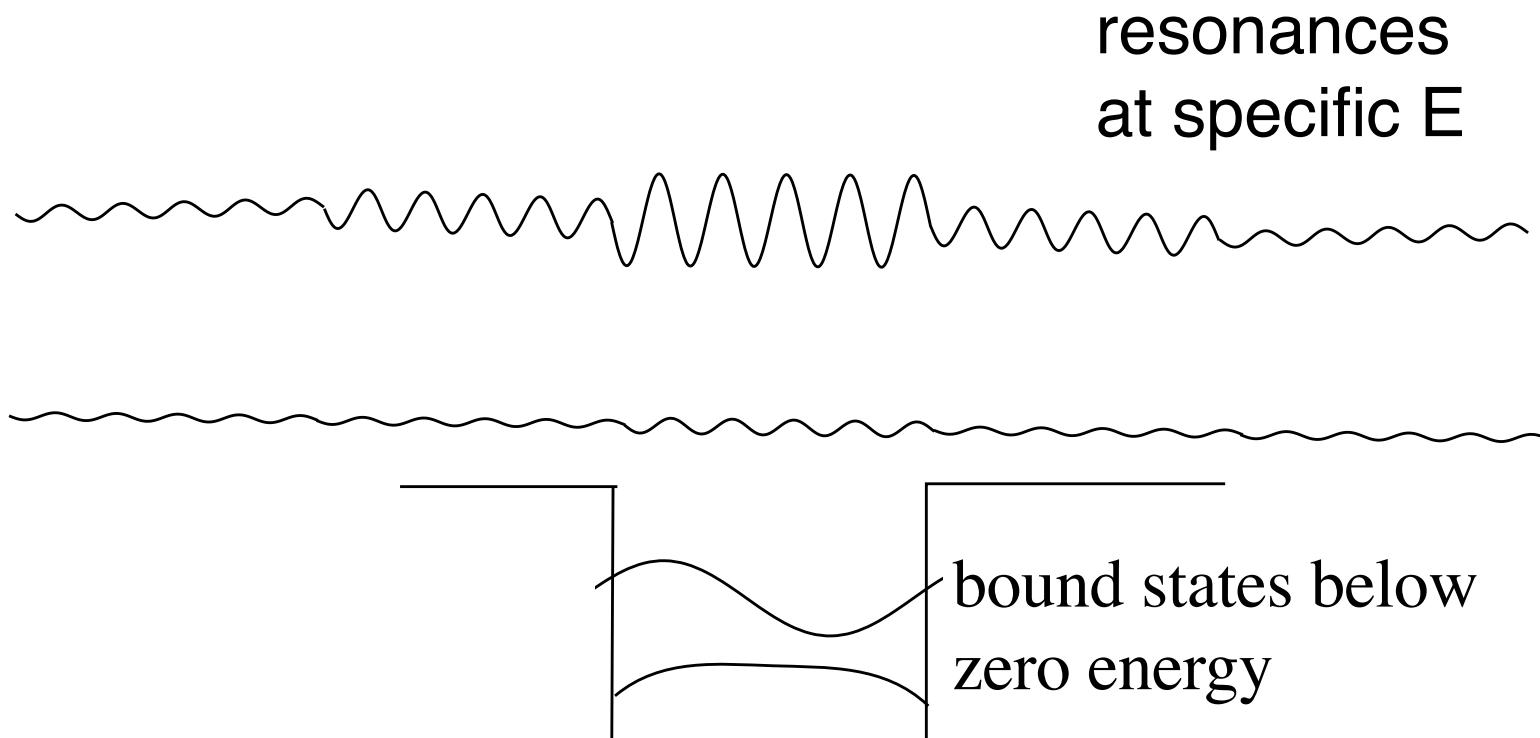
LB94: HOMO F⁻ = 3.48 eV ; IP = 3.40 eV

B-GLLB-VWN, see Amati, Baerends JCTC 16 (2020) 443:

Many closed shell anions: MAE + 0.14 eV

Many open shell anions: MAE + 0.48 eV

What is the meaning of an orbital with positive orbital energy?



What is the meaning of KS orbital energies?

Prevailing view on **occupied** orbital energies:
”..one should expect no simple physical
meaning for the KS orbital energies. *There is
none.*”

WRONG!

Prevailing view on **virtual** KS orbital energies:
The HOMO-LUMO gap is too low
(the “band gap” problem of KS DFT)

WRONG!

KS HOMO-LUMO gaps Δ are excellent approx. to excitation energies

	Δ^{HF}	Δ^{LDA}	Δ^{BLYP}	Δ^{KS}	Expt. excit. energy singlet	Expt. excit. energy triplet
H ₂	17.6	10.6	10.5	12.5	12.7	11.7
H ₂ O	14.7	6.5	6.2	7.5	7.65	7.5
HF	18.5	8.9	8.5	10.5	10.3	9.9
N ₂	19.9	9.7	9.6	9.9	9.3-10.3	7.8-8.9
CO	17.0	6.9	7.1	7.5	8.5	6.3
HCN	15.4	7.9	7.8	8.0	8.8	6.2
FCN	14.8	7.3	7.0	7.6	8.4	7.8
HCl	13.8	7.0	6.8	7.4	7.8	7.4

- 1) The LDA, GGA gaps (aug-cc-pVTZ basis) are similar (slightly smaller) than KS gaps
-> the upshift is similar for HOMO and (a bit smaller for) LUMO
- 2) HF gaps are much larger: Koopmans' approx. to IP – EA if ϵ_{LUMO} neg.
Many HF LUMOs at positive orbital energy!

HF, DFA and exact KS LUMO orbital energies

	HF	LDA	BLYP	KS
H ₂	+1.42	+0.31	+0.12	-3.93
H ₂ O	+0.80	-0.92	-1.06	-5.11
HF	+0.81	-0.93	-1.13	-5.71
N ₂	+3.91	-2.21	-1.91	-6.77
CO	+1.88	-2.24	-1.94	-6.56
HCN	+1.93	-1.33	-1.07	-5.53
FCN	+1.16	-1.66	-1.59	-6.01
HCl	+0.79	-1.11	-1.15	-5.36

KS LUMO is at negative energy: a bound one-electron state in the KS potential.

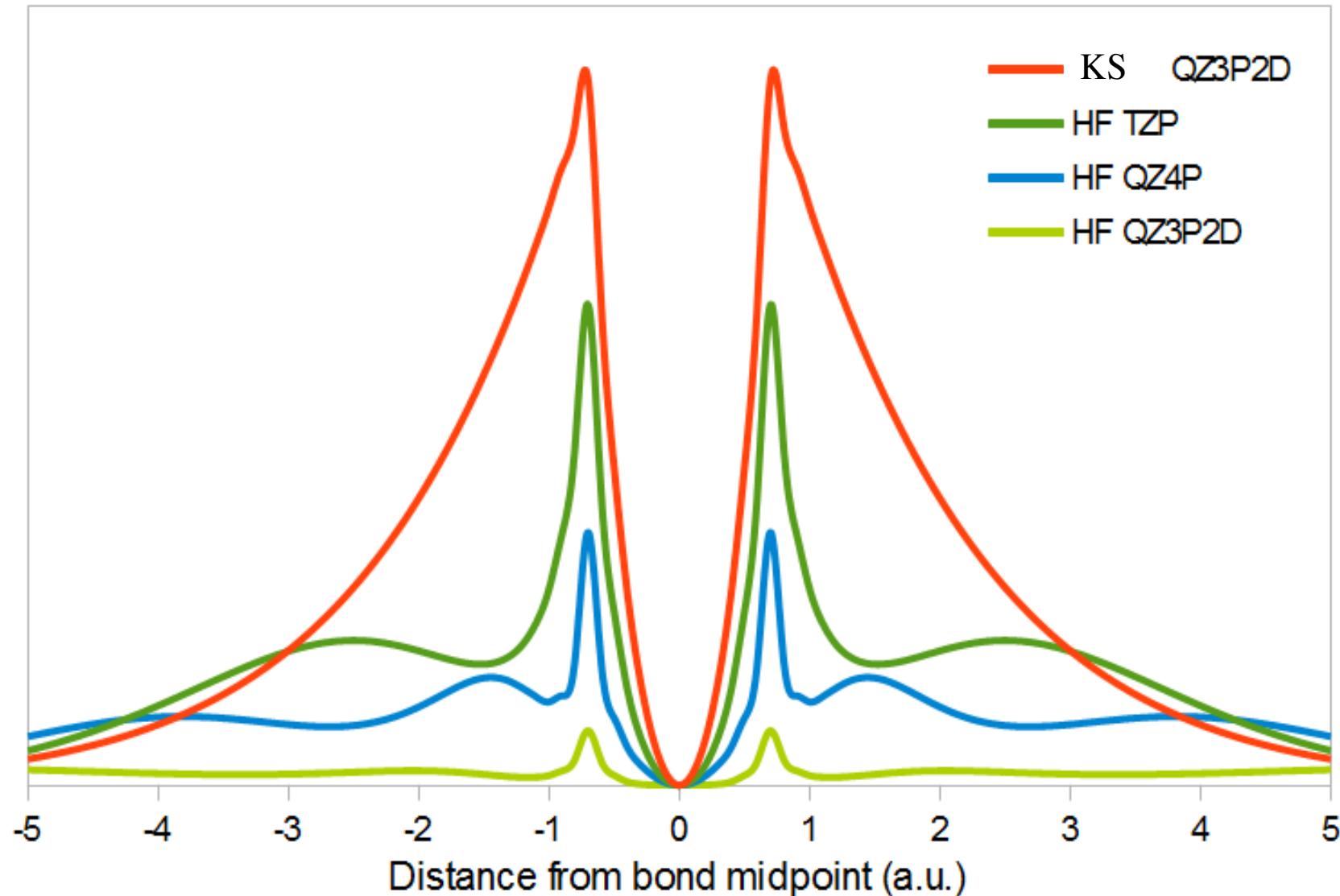
HF LUMO is most of the time *unbound* (positive orbital energy)

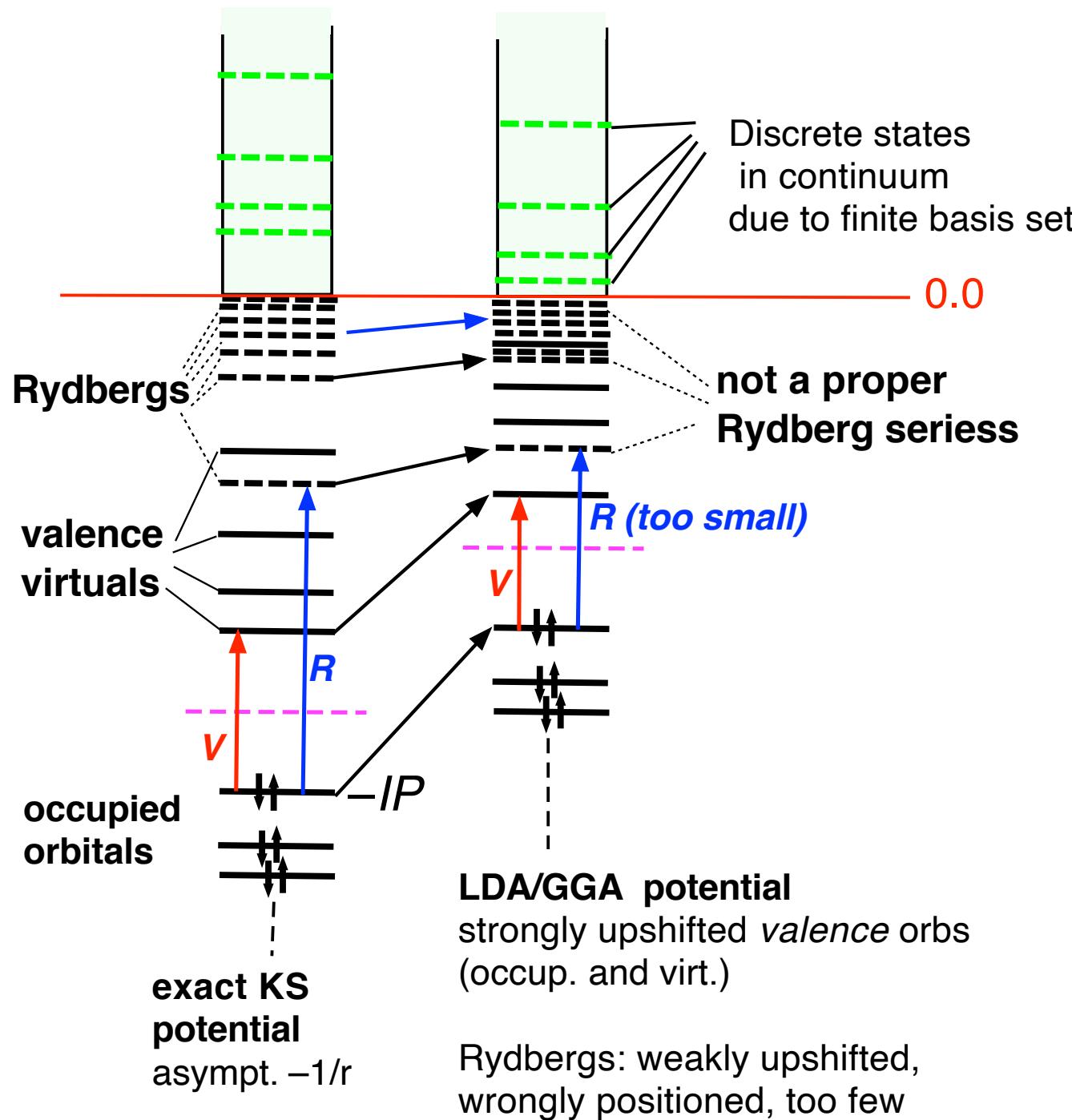
LDA, GGA LUMO: still negative -> therefore bound state

Orbital energies (eV) of the positive energy HF LUMO of H₂ as function of the basis (STOs)

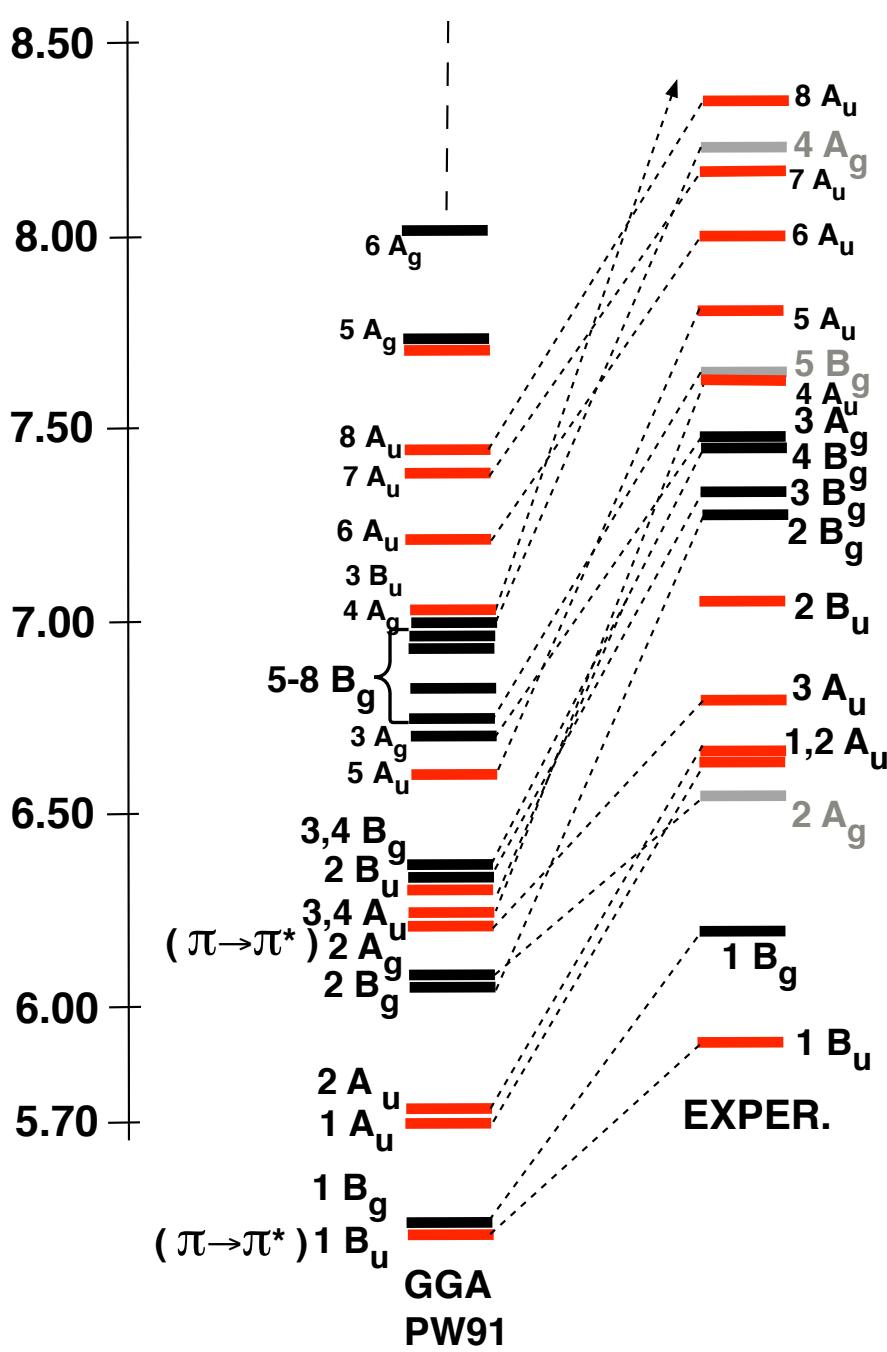
	SZ	DZ	DZP	TZP	TZ2P	QZ4P	ETQZ3P 2D
1σ _u	18.12	5.52	5.11	3.39	3.45	2.67	1.18
1σ _g	-15.88	-16.26	-16.20	-16.21	-16.20	-16.18	-16.18
gap	34.00	21.77	21.31	19.59	19.66	18.85	17.36

Shape of the $1\sigma_u$ LUMO density of H_2 as a function of basis set:





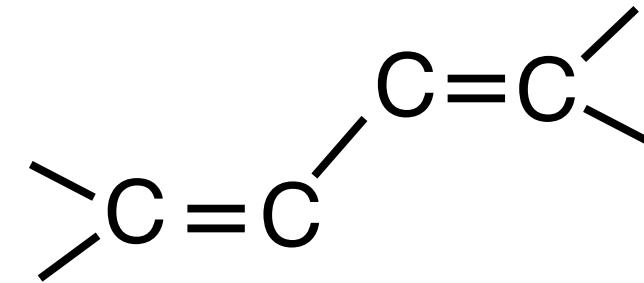
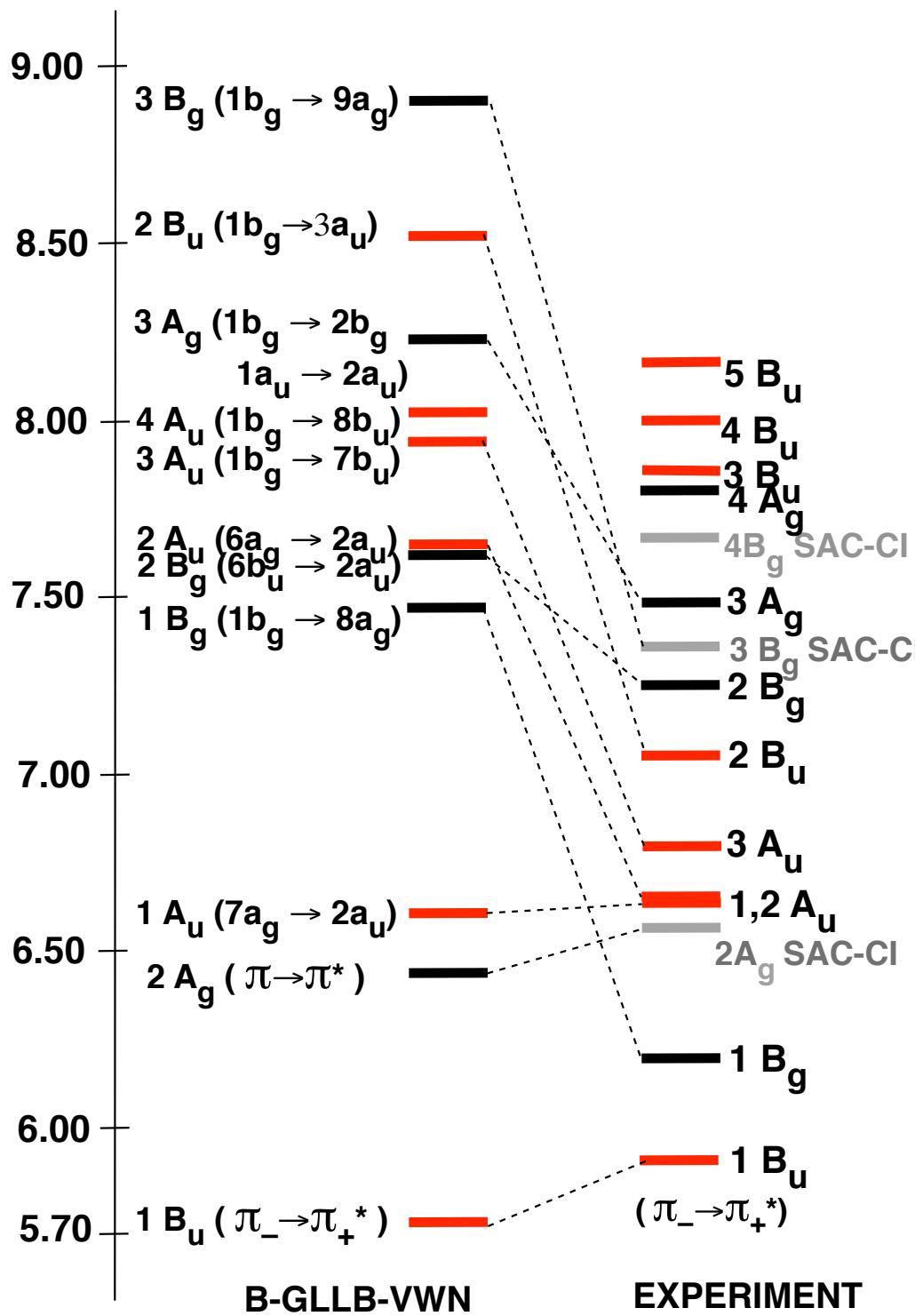
proper
KS pot.
important
for *virtual*
orbital
spectrum!



For TDDFT it is essential to have
orbitals and orbital energies
from good approx. to exact KS potential

→ B-GLLB-VWN!

- good occupied and virtual orbital energies
 - from B88 correction to LDA proper $-1/r$
asymptotics of potential expected
- Rydbergs OK?



Vertical excitations
 1,3-transbutadiene
 TDDFT with
 B-GLLB-VWN approx. to
 exact KS potential
 + ALDA kernel

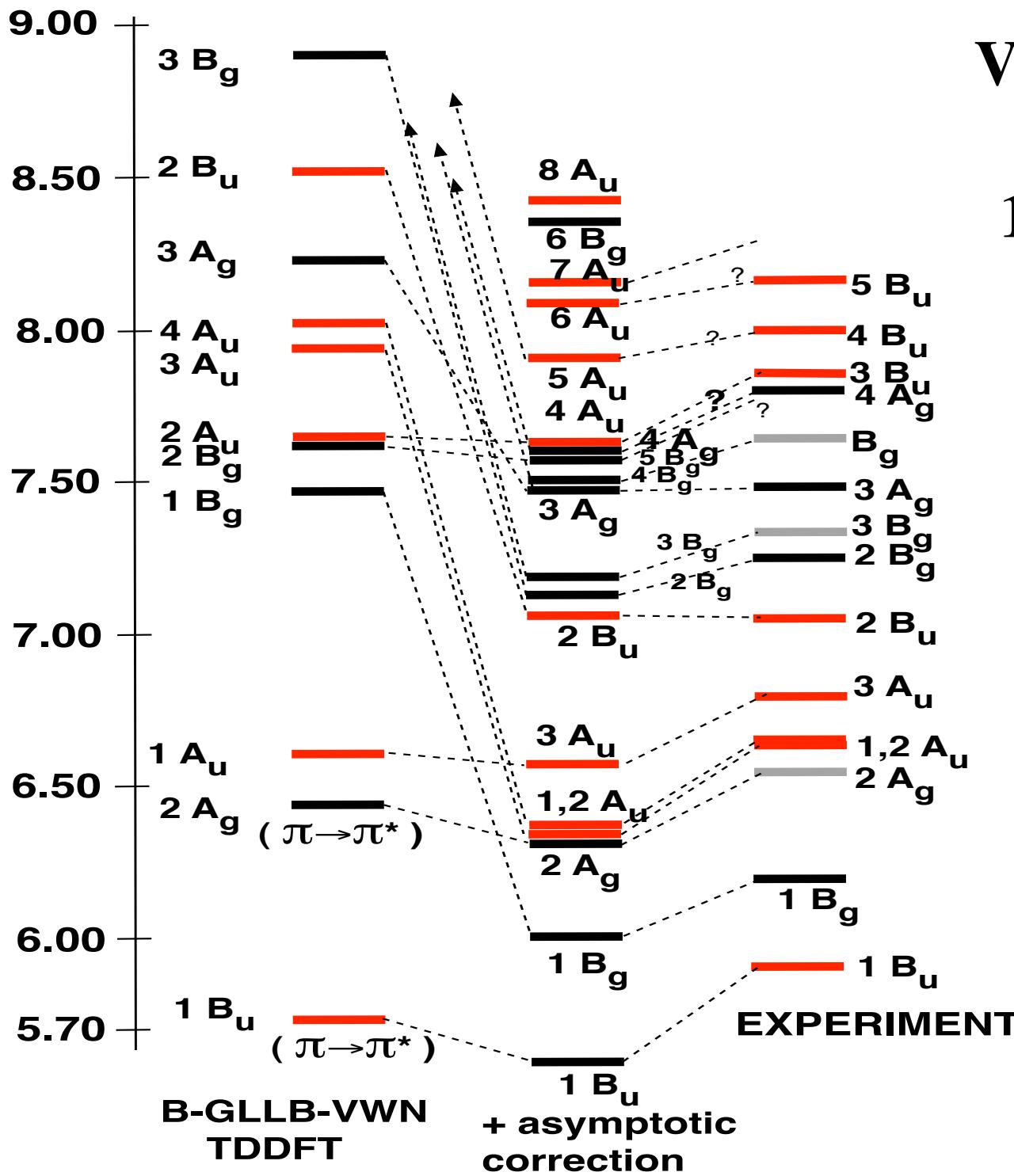
poor!
Rydbergs too much
upshifted
-> asymptotics of
potential not right?

Why such poor TDDFT results with B-GLLB-VWN potential?

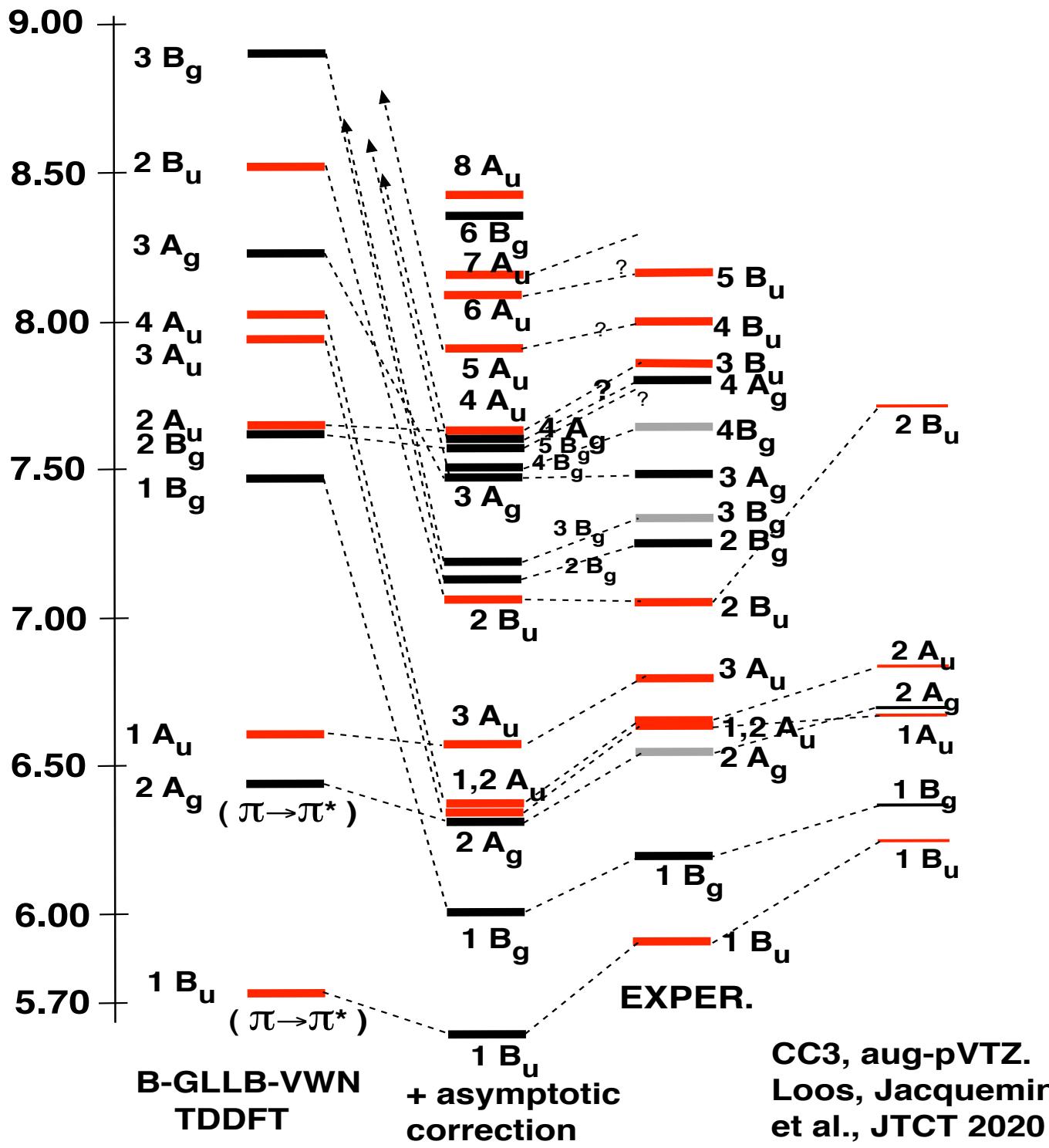
Possibly due to deficient long range / asymptotic behavior of potential,
in spite of $-1/r$ asymptotics coming from B88 energy density ?

Test: add asymptotic behavior of LB94 KS potential
(R. van Leeuwen, E. J. Baerends, PRA 1994)

Vertical excitation
energies (eV)
1,3-transbutadiene
with
proper
asymptotics

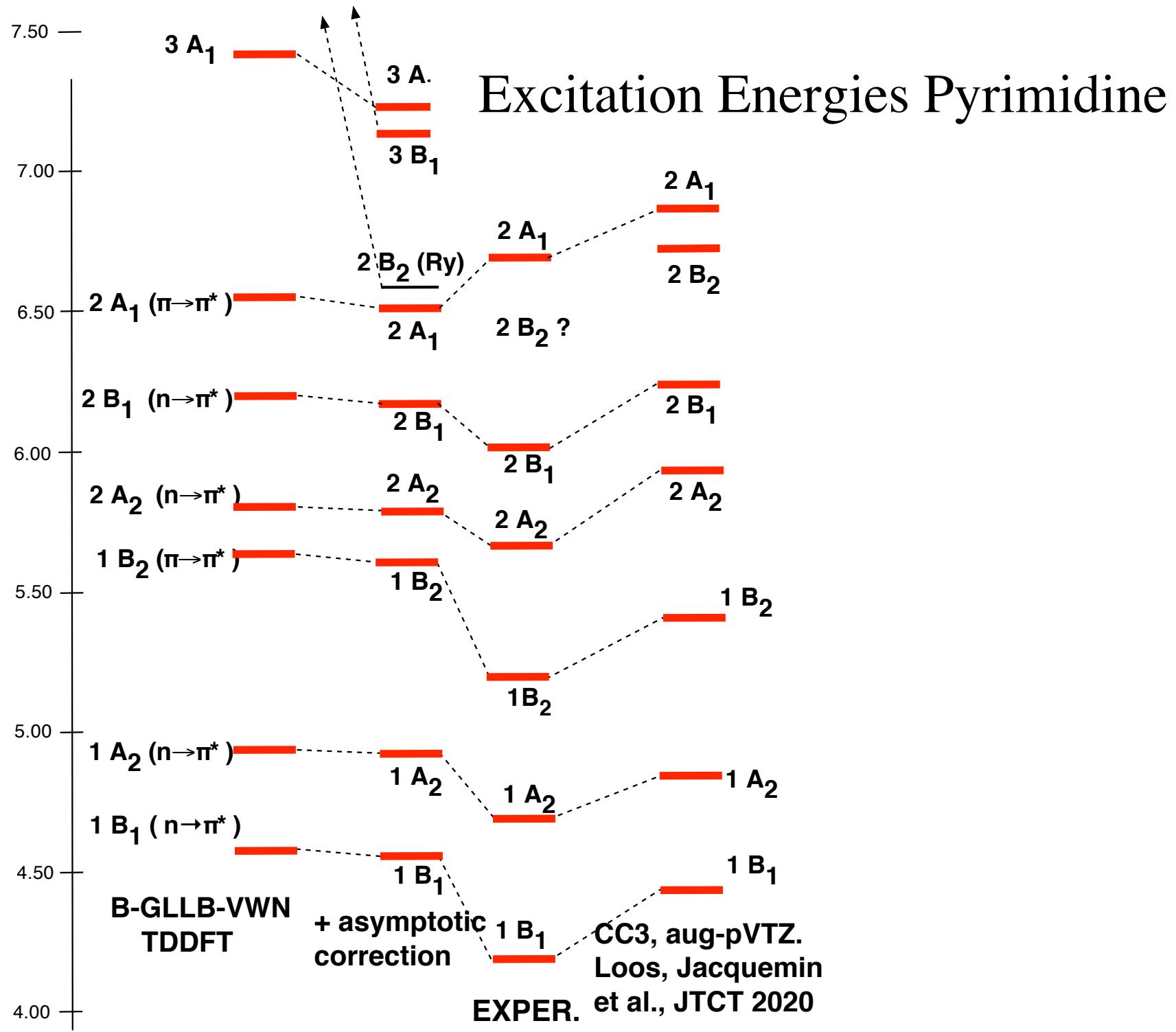


Compare to CC



Excitations 1,3-transbutadiene, best theoretical results

	6-31G(d) CC3	aug-cc-pVTZ				th.	th.	EXP.
	CC3	CC3	CCSDT	NEV- PT2	SAC-CI	MR- AQCC		
B_u	6.41	6.22	6.24	6.68	6.33	6.36		5.92
B_g	6.53	6.33	6.34	6.44	6.18	6.32		6.21
A_u	6.87	6.64	6.66	6.84	6.45	6.56		6.64
A_g	6.73	6.67	6.60	6.70	6.56	6.50		
A_u	6.93	6.80	6.81	7.01	6.65	6.74		6.80
B_u	7.98	7.68	-	7.45	7.08	7.02		7.07



Acetone: orbital en. differences and excit. energies (eV)

Funct.	State	Weight	ε_i	ε_a	$\Delta\varepsilon_{ia}$	ω_{TD-DFT}	$\omega - \Delta\varepsilon_{ia}$	$\omega - E_{exp}$
	1A₂	1.00	-10.25	-5.92	4.33	4.59	0.26	0.16
“exact” KS pot.	1B₂	1.00	-10.25	-4.18	6.07	6.09	0.02	-0.27
(SAOP)	2A₂	0.84	-10.25	-2.72	7.53	7.52	0.00	0.16
	2A₁	0.97	-10.25	-3.09	7.16	7.21	0.05	-0.20
	2B₂	0.97	-10.25	-2.63	7.62	7.64	0.02	0.15
	3A₁	0.97	-10.25	-2.04	8.21	8.20	0.00	0.40
	3B₂	0.97	-10.25	-2.51	7.74	7.74	0.00	-0.35
	1B₁	0.95	-10.25	-5.92	7.92	8.17	0.24	0.00

Acetone: orbital en. differences and excit. energies (eV)

Funct.	State	Weight	ε_i	ε_a	$\Delta\varepsilon_{ia}$	ω_{TD-DFT}	$\omega - \Delta\varepsilon_{ia}$	$\omega - E_{exp}$
BP86	1A₂	1.00	-5.71	-1.70	4.01	4.27	0.26	-0.16
	1B₂	1.00	-5.71	-0.61	5.10	5.10	0.00	-1.26
	2A₂	1.00	-5.71	-0.11	5.60	5.59	0.00	-1.77
	2A₁	1.00	-5.71	-0.13	5.58	5.58	0.00	-1.83
	2B₂	1.00	-5.71	-0.07	5.64	5.64	- 0.01	-1.85
	3A₁	0.98	-5.71	+0.36	6.07	6.06	- 0.01	-1.74
	3B₂	1.00	-5.71	+0.05	5.76	5.75	0.00	-2.34
	1B₁	1.00	-5.71	+0.31	6.02	6.01	-0.01	-2.16

Acetone: orbital en. differences and excit. energies (eV)

Funct.	State	Max. Weight	ε_i	ε_a	$\Delta\varepsilon_{ia}$	ω_{TD-DFT}	$\omega - \Delta\varepsilon_{ia}$	$\omega - E_{exp}$
TDHF	1A₂	0.47	-11.23	+3.96	15.18	5.03	-10.15	0.60
	1B₂	0.36	-11.23	+0.62	11.85	8.24	-3.61	1.88
	2A₂	0.43	-11.23	+1.02	12.25	9.02	-3.23	1.66
	2A₁	0.20	-11.23	+0.96	12.19	9.07	-3.12	1.66
	2B₂	0.31	-11.23	+1.20	12.43	9.13	-3.30	1.64
	3A₁	0.21	-11.23	+3.96	17.15	9.41	-7.74	1.61
	3B₂	0.23	-11.23	+1.74	12.96	9.59	-3.37	1.50
	1B₁	0.84	-11.23	+1.12	12.35	9.89	-2.46	1.72

Acetone: orbital energy differences and excitation energies (eV)

Funct.	State	Max. Weight	ε_i	ε_a	$\Delta\varepsilon_{ia}$	ω_{TD-DFT}	$\omega - \Delta\varepsilon_{ia}$	$\omega - E_{exp}$
M06-2X	1A ₂	0.52	-8.85	+0.78	9.63	4.03	-5.60	-0.40
	1B ₂	0.73	-8.85	-0.34	8.51	6.54	-1.97	0.18
	2A ₂	0.62	-8.85	+0.04	8.88	7.33	-1.55	-0.03
	2A ₁	0.62	-8.85	+0.03	8.87	7.38	-1.49	-0.03
	2B ₂	0.45	-8.85	+0.15	9.00	7.40	-1.60	-0.09
	3A ₁	0.79	-8.85	+0.74	9.58	8.03	-1.55	0.23
	3B ₂	0.42	-8.85	+0.64	9.49	7.80	-1.69	-0.29
	1B ₁	0.92	-8.85	+0.73	9.58	8.12	-1.45	-0.05

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