Adiabatic Connection Correlation Functional from Hartree-Fock Orbitals

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Outline

1. *Adiabatic Connection Integrand Interpolation* (ACII) Models in Density Functional Theory

2. *Møller-Plesset Adiabatic Connection* (MPAC)

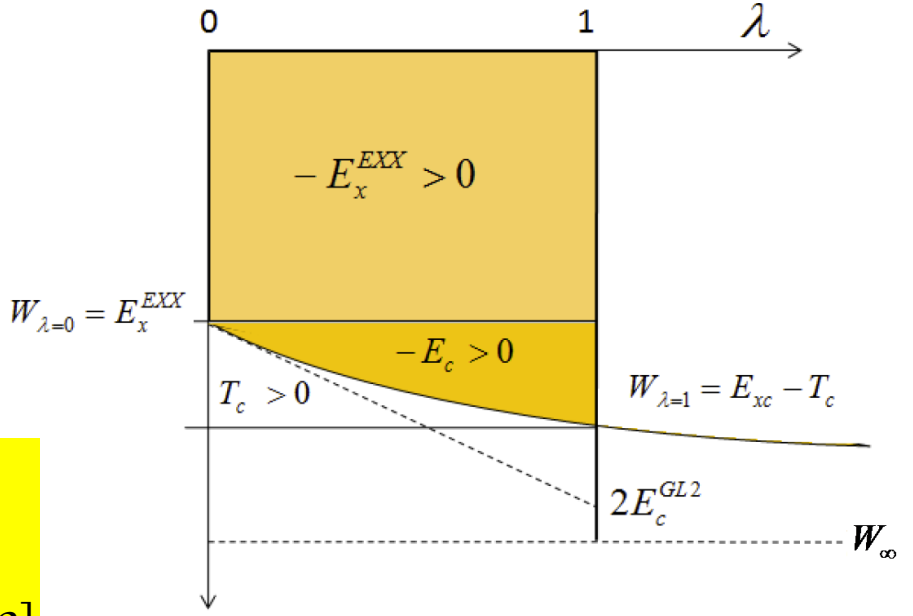
3. *HFAC24:* Construction and results

4. *AC* methods with FHI-aims

1. ACII (DFT)

XC functionals based on ACM

	DFT Adiabatic Connection
$\hat{H}_\lambda$	$\hat{T} + \hat{V}_{\text{ext}} + \lambda \hat{V}_{\text{ee}} + \hat{V}_\lambda[\rho]$
$\rho_{\lambda=0}$	ρ →**KS system** $V_{\lambda=0} = v_{xc}$
$\rho_{\lambda=1}$	ρ →**real system** $V_{\lambda=1} = 0$



$$E_{xc}[\rho] = \int_0^1 W_{xc}^\lambda[\rho] d\lambda$$

with $W_{xc}^\lambda[\rho] = \langle \Psi_\lambda[\rho] | \hat{V}_{ee} | \Psi_\lambda[\rho] \rangle - J[\rho]$

The AC method has been used to construct many XC functionals of different rungs

The AC integrand W_λ is not known explicitly, but it can be modeled by interpolating between the known asymptotic limits:

$$W_{xc}^\lambda[\rho] \xrightarrow[\lambda \to 0]{} E_x^{EXX} + 2\lambda E_c^{GL2} + O(\lambda^2)$$

$$W_{xc}^\lambda[\rho] \xrightarrow[\lambda \to \infty]{} W_\infty[\rho] + \frac{W'_\infty}{\sqrt{\lambda}} + \ldots$$

λ→∞ strong interaction limit

⇒**Adiabatic Connection Integrand Interpolation (ACII) methods use only $E_x^{EXX}, E_c^{GL2}, W_\infty, W'_\infty$ as ingredients.**

The ACII functional is defined by the interpolation formula

ACII methods ingredients

E_x^{EXX} (exact exchange) and
E_c^{GL2} are readily available in most quantum chemistry package

$$E_c^{GL2} = -\frac{1}{4}\sum_{abij}\frac{|\langle\phi_i\phi_j||\phi_a\phi_b\rangle|^2}{\epsilon_a+\epsilon_b-\epsilon_i-\epsilon_j}$$

MP2 with DFT orbitals

$$-\sum_{ia}\frac{|\langle\phi_i|\hat{v}_x^{KS}-\hat{v}_x^{HF}|\phi_a\rangle|^2}{\epsilon_a-\epsilon_i}$$

Singly excited term (very small)

Approximated GL2 from DFT:

$$E_c^{GL2} = \lim_{\lambda\to 0} E_c^{DFT}[\rho_{1/\lambda}]$$

used in MCY06 and others, not in this work

The strong interaction ingredients can be obtained from the Strictly Correlated Electron (SCE) method, or approximated as GGA density functionals

PC model:

$$W_\infty[\rho] = \int\left[A\rho(\mathbf{r})^{4/3} + B\frac{|\nabla\rho(\mathbf{r})|^2}{\rho(\mathbf{r})^{4/3}}\right]d\mathbf{r}$$

$$W'_\infty[\rho] = \int\left[C\rho(\mathbf{r})^{3/2} + D\frac{|\nabla\rho(\mathbf{r})|^2}{\rho^{7/6}(\mathbf{r})}\right]d\mathbf{r}$$

A,B,C fixed parameters
D depends of the model

Seidl, Perdew, Kurth, PRA 62, 12502 (2000)

hPC model:

$$W_\infty^{hPC} = \int d^3\mathbf{r}\, A\rho^{4/3}\left[\frac{1+s^2\mu_w\frac{\kappa_w+1}{\kappa_w}}{1+s^2\mu_w/\kappa_w}\right]$$

$$W_\infty^{\prime hPC} = \int d^3\mathbf{r}\, C\rho^{3/2}\left[\frac{1+s^2\mu_{w'}\frac{\kappa_{w'}+1}{\kappa_{w'}}}{1+s^2\mu_{w'}/\kappa_{w'}}\right]$$

κ_W

$\kappa_{W'}$

Fitted on Hooke's atom

Śmiga, Della Sala, Gori-Giorgi, Fabiano JCTC 18, 5936 (2022)

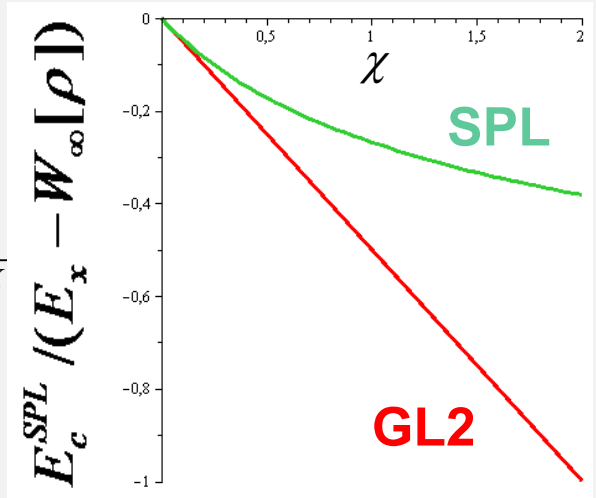
Earliest ACII

$$E_{xc} = f^{ACM}(E_x^{EXX}, E_c^{GL2}, W_\infty)$$ **SPL, LB**

SPL: Seidl, Perdew, Levy, PRA 59, 51 (1999)
LB: Liu, Burke, PRA 79,064503 (2009)

$$W_\lambda^{SPL} = W_\infty[\rho] + \frac{E_x^{EXX} - W_\infty[\rho]}{\sqrt{1+2\lambda\chi[\rho]}}; \quad \chi = \frac{2E_c^{GL2}}{W_\infty - E_x^{EXX}}$$

$$E_{xc}^{SPL} = E_x^{EXX} + (E_x^{EXX} - W_\infty)\left(\frac{\sqrt{(1+2\chi}-1-\chi}{\chi}\right)$$



GL2 overestimates the correlation, SPL corrects it

$$E_{xc} = f^{ACM}(E_x^{EXX}, E_c^{GL2}, W_\infty, W'_\infty)$$

ISI (Interaction Strength Interpolation)
revISI

ISI: Seidl, Perdew, Kurth, PRL 84, 5070 (2000)
revISI: Gori-Giorgi, Vignale, Seidl, JCTC 5,743 (2009)

$$W_\lambda^{ISI} = W_\infty[\rho] + \frac{X[\rho]}{\sqrt{1+Y[\rho]\lambda + Z[\rho]}} \qquad X = -\frac{4E_c^{GL2}(W'_\infty)^2}{(E_x - W_\infty)^2}; \; Y = \frac{16(E_c^{GL2})^2(W'_\infty)^2}{(E_x - W_\infty)^4}; \; Z = -\frac{4E_c^{GL2}(W'_\infty)^2}{(E_x - W_\infty)^3} - 1$$

$$E_{xc}^{ISI} = W_\infty + \frac{2X}{Y}\left[\sqrt{1+Y} - 1 - Z\ln\left(\frac{\sqrt{1+Y}+Z}{1+Z}\right)\right],$$

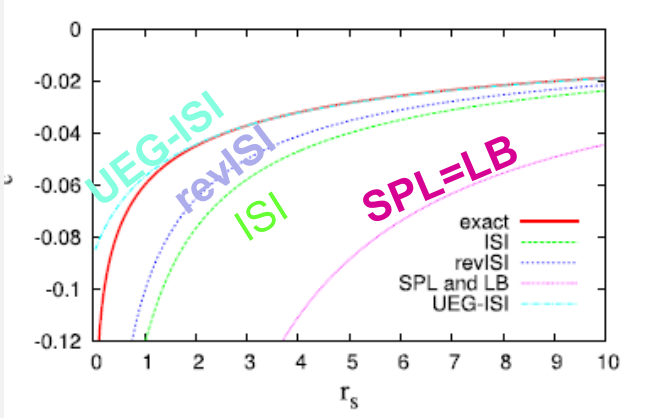
Recent ACII

UEG-ISI: AC limit for EGL2 = −∞

$$W_{xc,\alpha}^{UEG-ISI}[n] = W_\infty[n] + \frac{b(2 + c\alpha + 2d\sqrt{1+c\alpha})}{2\sqrt{1+c\alpha}(d+\sqrt{1+c\alpha})^2}$$

$$b[n] = (E_x^{EXX} - W_\infty)(1+d) \qquad c[n] = b[n]^2/[4W_\infty'^2].$$

DPI (exact for UEG)



UEGISI well reproduces the UEG correlation energies for rs>1.

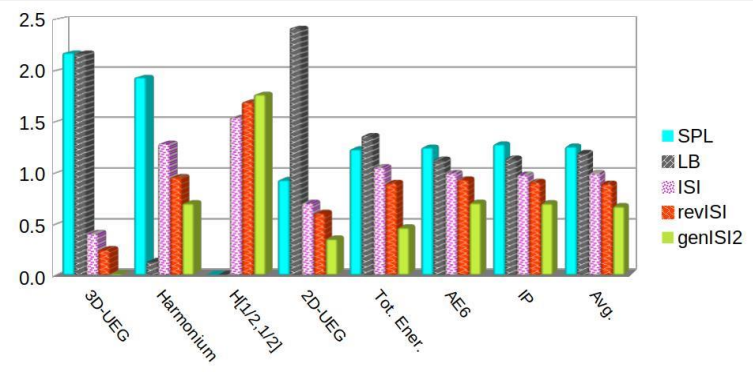
Constantin, Jana, Śmiga, Della Sala, JCP 159, 244111 (2023)

genISI2

$$W_{xc,\lambda}^{genISI2} = W_{xc,\lambda}^{UEG-ISI}[n] + \frac{2E_c^{GL2}\lambda}{\left(1 + l_1 r[n]\frac{2E_c^{GL2}}{E_x^{EXX}}\lambda\right)^3} + \frac{-W_{xc,\lambda}^{UEG-ISI}[n] + E_x^{EXX}}{\left(1 + l_2 r[n]\frac{2E_c^{GL2}}{E_x^{EXX}}\lambda\right)^3}$$

with $r[n] = \left(\frac{E_x^{EXX}}{W_\infty}\right)^3$

$$W_{xc,\lambda}^{genISI2} \underset{\lambda\to 0}{\to} E_x^{EXX} + 2E_c^{GL2}\lambda$$



Broad applicability

Constantin, Śmiga, Della Sala, PRB 190, 23519 (2024)

ACII vs Double Hybrid

ACII: $E_{xc} = f^{ACM}(E_x^{EXX}, E_c^{GL2}, W_\infty, W'_\infty)$

Double hybrid: $E_{xc}^{DH} = \alpha E_x^{EXX} + \beta E_c^{MP2} + (1-\alpha)E_x^{DFT} + (1-\beta)E_c^{DFT}$

ACII models are computationally similar to double hybrids, but

- 😐 **are NOT LINEAR in MP2**
- 🙂 **have always full exact exchange (no error compensation)**
- 🙂 **do not diverge for metals (in contrast to DH)**

Limitations of DFT ACII methods

- GL2 energy strongly dependent on the ground-state orbitals

Neon Atom	E_x^{EXX}	W_∞	W'_∞	E_c^{GL2}	Gap
CCSD(T)	−12.078	−20.051	23.041	−0.4741	17.12
S-VWN	−12.008 (−0.6%)	−19.964 (−0.4%)	22.952 (−0.4%)	−0.499 (+5.3%)	15.53
PBE	−12.044 (−0.3%)	−20.011 (−0.2%)	23.016 (−0.1%)	−0.491 (+3.6%)	15.15
HF	−12.108 (+0.2%)	−20.076 (+0.1%)	23.045 (0%)	−0.367 (−22.6%)	27.39
OEPx	−12.104 (+0.2%)	−20.078 (+0.1%)	23.044 (0%)	−0.4631(−2.3%)	18.44

- OEP-SCF calculations possible, but expensive

Śmiga, Della Sala, Gori-Giorgi, Fabiano JCTC 18, 5936 (2022)

2. MPAC

MPAC are based on Hartree-Fock orbitals.

MPAC thus resembles Post-HF correlation methods or the density-corrected DFT (DC-DFT)

MP-adiabatic connection (MPAC)

	Møller-Plesset Adiabatic Connection
$\hat{H}_\lambda$	$\hat{T} + \hat{V}_{\text{ext}} + \hat{V}^{\text{HF}} + \lambda\left(\hat{V}_{\text{ee}} - \hat{V}^{\text{HF}}\right)$
	$\hat{V}^{\text{HF}} = \hat{J}[\rho^{\text{HF}}] - \hat{K}[\{\phi_i^{\text{HF}}\}]$
$\rho_{\lambda=0}$	ρ^{HF}
$\rho_{\lambda=1}$	ρ
ρ_λ	ρ_λ

Density is not fixed

$$W_{\lambda\to 0}^{\text{HF}} = E_x^{\text{HF}} + 2E_c^{MP2}\lambda + \ldots$$

$$W_{\lambda\to\infty}^{\text{HF}} = W_\infty^{\text{HF}} + \frac{1}{\sqrt{\lambda}} W_\infty'^{\text{HF}} + \cdots$$

Rewriting of the Many-body correlation

$$E_{xc}^{\text{HF}} = \int_0^1 W_\lambda^{\text{HF}}\, d\lambda$$

$$W_\lambda^{\text{HF}} \equiv \langle \Psi_\lambda^{\text{HF}} | \hat{V}_{ee} - \hat{J} - \hat{K} | \Psi_\lambda^{\text{HF}} \rangle + U[\rho^{\text{HF}}] + 2E_x^{\text{HF}}$$

Seidl, Gianrusso, Vuckovic, Gori-Giorgi JCP 149 ,241101 (2018)

$\lambda\to\infty$ strong interaction limit MPAC functionals: gradient expansion as in DFT

$$W_\infty^{\text{HF}} = A^{\text{HF}} \int \mathrm{d}\mathbf{r}\, \rho(\mathbf{r})^{4/3} + B^{\text{HF}} \int \mathrm{d}\mathbf{r}\, \frac{|\nabla\rho(\mathbf{r})|^2}{\rho(\mathbf{r})^{4/3}} + \boldsymbol{E_x^{HF}}$$

$$W_\infty'^{\text{HF}} \approx C^{\text{HF}} \int \mathrm{d}\mathbf{r}\, \rho(\mathbf{r})^{3/2} + D^{\text{HF}} \int \mathrm{d}\mathbf{r}\, \frac{|\nabla\rho(\mathbf{r})|^2}{\rho(\mathbf{r})^{7/6}}$$

Daas et al, JCTC 18, 5164 (2022)

Initial attempts: MPAC for dispersion systems

SPL2

$$W_{c,\lambda}^{\mathrm{SPL2}} = C_1 - \frac{m_1}{\sqrt{1 + b_1\lambda}} - \frac{m_2}{\sqrt{1 + b_2\lambda}}$$

MPACF1

$$E_{c,\lambda}^{\mathrm{MPACF\text{-}1}} = -g\lambda + \frac{g(h+1)\lambda}{\sqrt{d_1{}^2\lambda + 1} + h\sqrt[4]{d_2{}^4\lambda + 1}}$$

MAE in kcal/mol

set	MP2	SPL	SPL2	MPACF-1	B3LYP-D3
NGD8	0.04	0.05	**0.03**	**0.03**	0.08
CT7	0.92	0.57	**0.45**	0.60	1.48
DI6	0.48	0.27	**0.18**	0.20	0.46
S22	0.88	0.38	**0.15**	0.19	**0.15**
S66	0.47	0.35	0.21	0.26	**0.18**
L7	8.74	3.83	**0.89**	2.32	1.78

Excellent accuracy (without any Dispersion correction!)

Low Computational costs: MP2 + DFT post-HF calculation

Empirical Parameters

Daas, Fabiano, Della Sala, Gori-Giorgi, Vuckovic, JPCL 12 , 4867 (2021)

Daas, Kooi, Peters, Fabiano, Della Sala, Gori-Giorgi, Vuckovic, JPCL 14, 8448 (2023)

3. HFAC24

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Letter

Nonempirical Adiabatic Connection Correlation Functional from Hartree–Fock Orbitals

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Construction of the HFAC24 functional

a) Definition of the strong-interaction functionals

$$W^{\mathrm{HF}}_{\mathrm{c},\alpha\to\infty}[n^{\mathrm{HF}}] \to W^{\mathrm{HF}}_{\mathrm{c},\infty}[n^{\mathrm{HF}}] + \frac{W^{\mathrm{HF}}_{1/2}[n^{\mathrm{HF}}]}{\alpha^{1/2}} + \frac{W^{\mathrm{HF}}_{3/4}[n^{\mathrm{HF}}]}{\alpha^{3/4}} + \cdots$$

$$E_{\mathrm{el}}[n^{\mathrm{HF}}] + E_x^{\mathrm{HF}}$$

$$E_{\mathrm{c}}^{\mathrm{HFAC24}} = \int_0^1 \mathrm{d}\lambda \left(2\lambda E_{\mathrm{c}}^{\mathrm{MP2}} G(\lambda E_{\mathrm{c}}^{\mathrm{MP2}}) + W_{\mathrm{c},\lambda}^{\mathrm{uegIHF}} (1 - G(\lambda E_{\mathrm{c}}^{\mathrm{MP2}}))\right)$$

b) Definition on W in the $E_{MP2}\to-\infty$ limit

c) Definition of the mixing function G

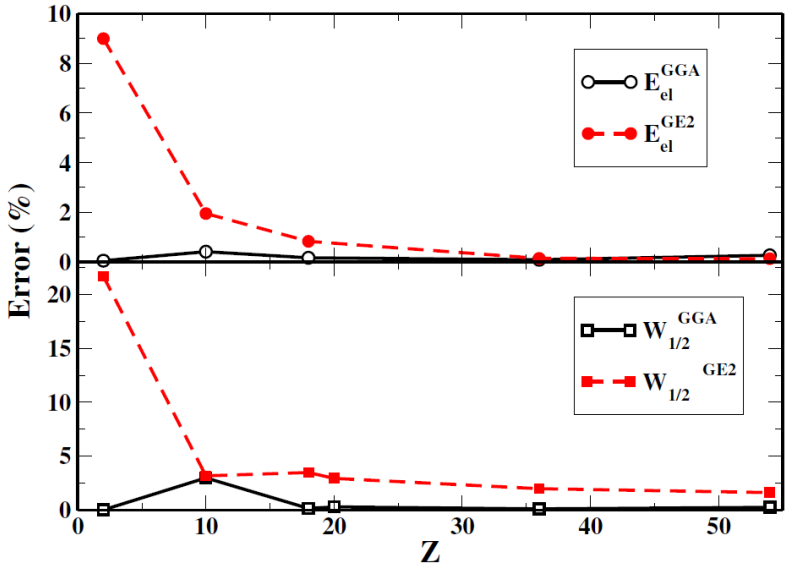
Constantin, Fabiano, Della Sala, JPChem Lett. 16, 3378 (2025)

HFAC24: part a, (strong-interaction)

GGA functional:

$$E_{el}^{GGA}[n] = A^{HF} \int d\mathbf{r}\, n(\mathbf{r})^{4/3} F_{el}(s)$$

$$W_{1/2}^{GGA}[n_\uparrow, n_\downarrow] = C^{HF} \int d\mathbf{r}\, n(\mathbf{r})^{3/2} F_w(s)(1 + \beta f(\zeta))$$



Functional not fitted to molecular systems (as DFT): functionals developed to reproduce strong-interaction regime in atoms

Constantin, Fabiano Della Sala, JPChem Lett. 16, 3378 (2025)

Spin function

$$W_{3/4}^{HF}[n_\uparrow, n_\downarrow] = \frac{(4\pi)^{1/4}}{4} \sum_k \epsilon_{3/4}(\sigma_{\mathbf{R}_k}) Z_k \rho^{HF}(\mathbf{R}_k)^{1/4} < 0$$

Density at the nuclei position !

Daas et al, JPCA 128 (2024) 4138

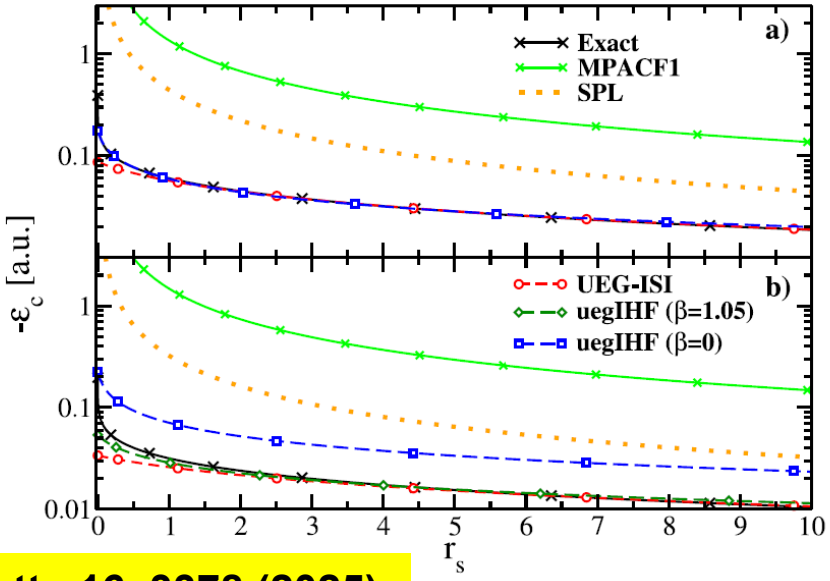
HFAC24: part b, (UEG)

$$W_{c,\alpha}^{\mathrm{uegIHF}}[n^{\mathrm{HF}}] = W_{c,\infty}^{\mathrm{HF}}[n^{\mathrm{HF}}]$$

$$+ \frac{b(2 + c\alpha + 2d_1\sqrt{\alpha c + 1})}{2\sqrt{\alpha c + 1}\,(d_2 + g(\alpha c + 1)^{1/4} + \sqrt{\alpha c + 1})^2}$$

$$b = b[n^{\mathrm{HF}}],\ c = c[n^{\mathrm{HF}}],\ \text{and}\ g = g[n^{\mathrm{HF}}]$$

Functional developed to reproduce the UEG



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HFAC24: part c, (mixing)

$$W_{c,\alpha}^{\mathrm{HFAC24}} = (2\alpha E_c^{\mathrm{MP2}})G(\alpha) + \\ + W_{c,\alpha}^{\mathrm{uegIHF}}[1 - G(\alpha)]$$

***K*=0.3 (to recover Helium atom correlation)**

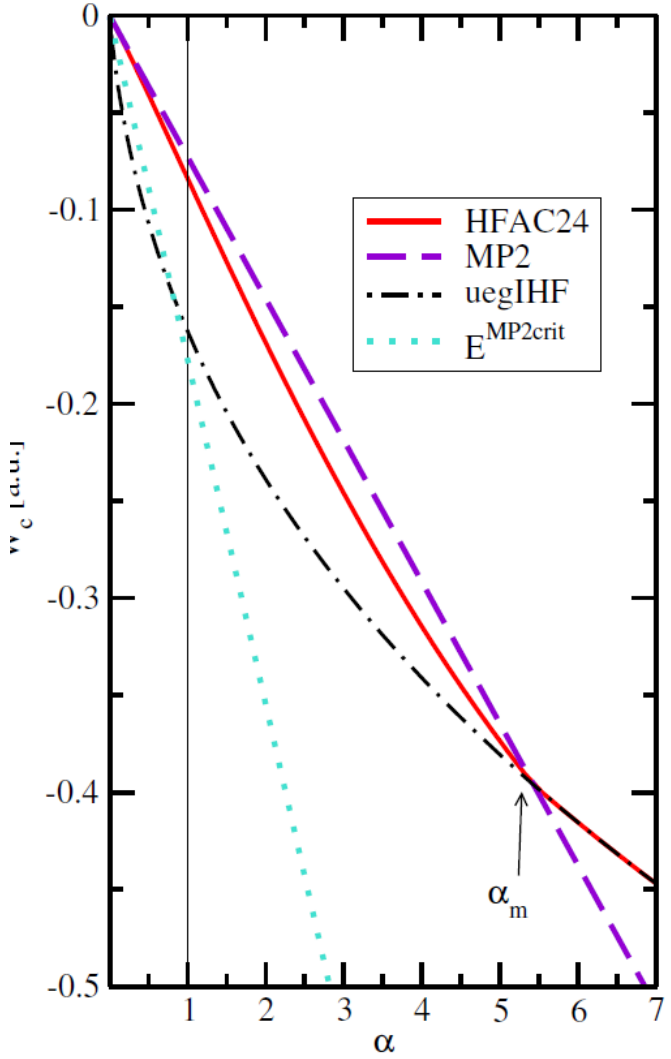
$$2\alpha E_c^{\mathrm{MP2}} > W_{c,\alpha}^{\mathrm{uegIHF}}$$

$$G(\alpha) = \mathrm{erfc}(\kappa\alpha E_c^{\mathrm{MP2}} / E_c^{\mathrm{uegIHF}})$$

Otherwise:

$$G(\alpha) = 0$$

E_c^{MP2}	E_c^{HFAC24}	systems
$E_c^{MP2crit} < E_c^{MP2}$	$E_c < E_c^{MP2}$	atoms and molecules
$E_c^S < E_c^{MP2} < E_c^{MP2crit}$	$E_c^{MP2} < E_c$	large atoms
$E_c^{MP2} < E_c^S$	$E_c = E_c^{uegIHF}$	strong correlation
$E_c^{MP2} = -\infty$	$E_c = E_c^{uegIHF}$	metals, zero-gap systems



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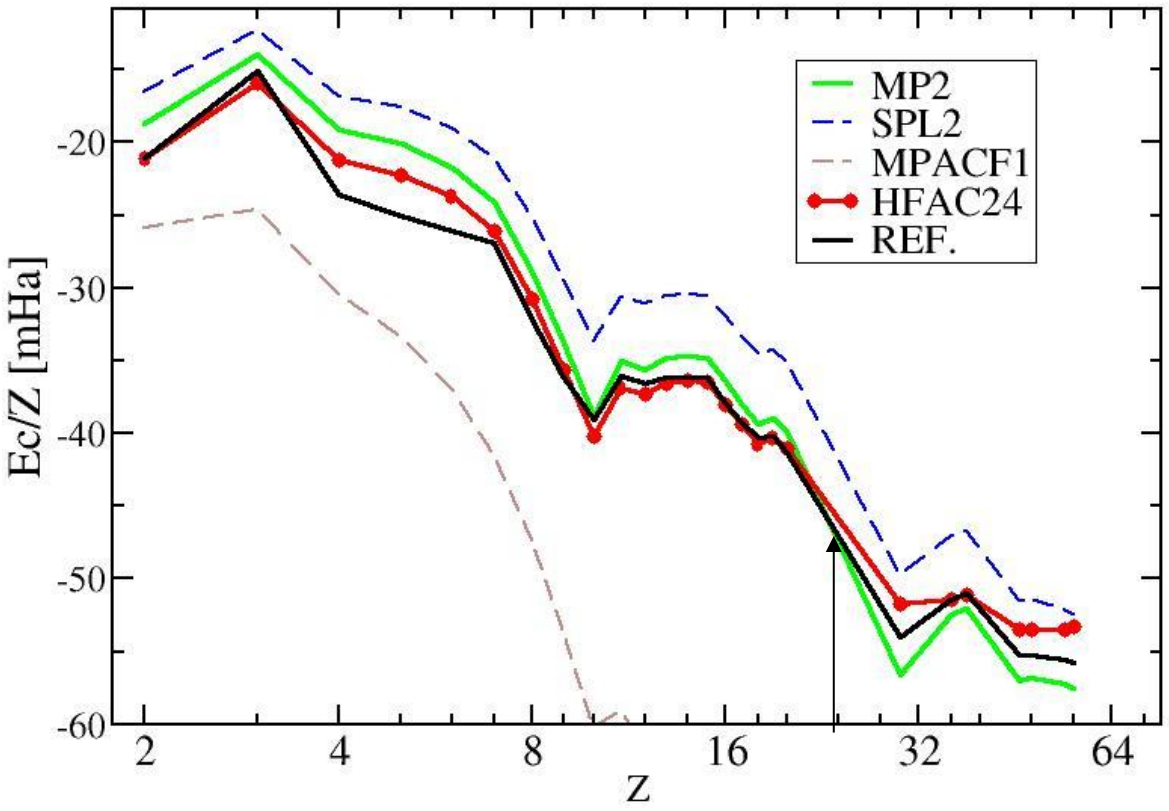
Results for Atomic correlation



High accuracy (1mHa per electron)

MP2 inversion at about Z=20

	PBE	TPSS	MP2	SPL	SPL2	MPACF1	HFAC24
				overall error statistics			
ME	-2.0	-1.8	-1.0	-3.4	-5.3	+34.0	-0.6	-2.8
MAE	2.2	2.0	1.9	3.4	5.3	34.0	**1.0**	2.8

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Molecular Benchmark

HFAC24 functional depends on EcMP2/EcUEG:

As EcUEG contains all-electron correlation, EcMP2 must do the same

CBS extrapolation or the 5ZaPaNR-CV basis-set is required

	Tot.Ener.	Atomiz.		Ener. Diff.		Electr. Bonds			Weak Bonds			
method	TE18	AE6	dimers	isomers	G21IP'	CT7	DI6	HB16	ngd	A24mt	A24di	LRMAE
					MAE							
PBED	75.60	14.45	7.28	3.20	3.98	3.13	0.99	1.24	0.10	0.40	0.24	0.96
TPSSD	35.20	**5.13**	**3.48**	3.35	4.06	2.58	0.68	0.79	0.08	0.18	**0.14**	0.47
B3LYPD	**9.80**	**4.86**	**2.69**	**1.87**	3.76	1.23	0.43	0.52	0.04	0.16	**0.13**	**-0.05**
B2PLYPD	18.70	**1.36**	**1.32**	**1.55**	**2.29**	0.79	**0.32**	0.33	0.03	0.10	0.17	**-0.30**
MP2	15.80	10.23	5.23	2.80	2.66	0.48	0.43	0.19	0.03	0.09	0.15	0.00
SOS-MP2	**13.90**	**5.12**	**3.00**	**0.99**	2.81	0.97	0.67	1.10	0.08	0.52	0.41	0.21
SCS-MP2	**14.00**	**5.40**	**2.61**	**1.42**	**2.52**	0.49	**0.34**	0.73	0.06	0.32	0.24	0.02
SPL	37.20	14.93	**4.97**	**2.04**	2.97	**0.24**	**0.15**	0.26	**0.02**	**0.08**	0.15	0.07
SPL2	53.90	20.77	6.70	**2.05**	3.47	**0.30**	**0.16**	0.25	**0.01**	**0.07**	**0.15**	0.18
MPACF1	233.00	21.33	9.91	**2.48**	3.38	**0.36**	**0.16**	**0.18**	**0.01**	**0.08**	0.16	0.54
HFAC24	**5.40**	**4.61**	**3.06**	**2.33**	**2.12**	**0.30**	**0.19**	0.36	0.04	0.10	**0.12**	**-0.42**

HFAC24 competitive with B2PLYPD !

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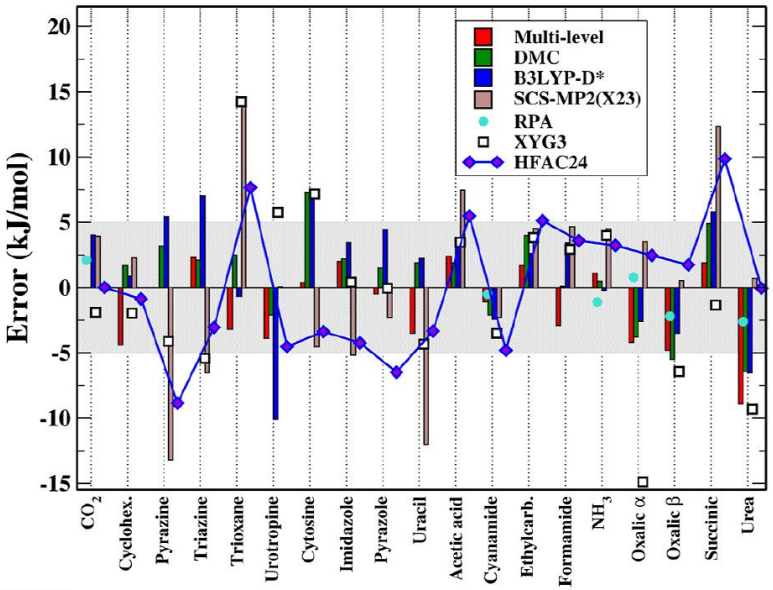
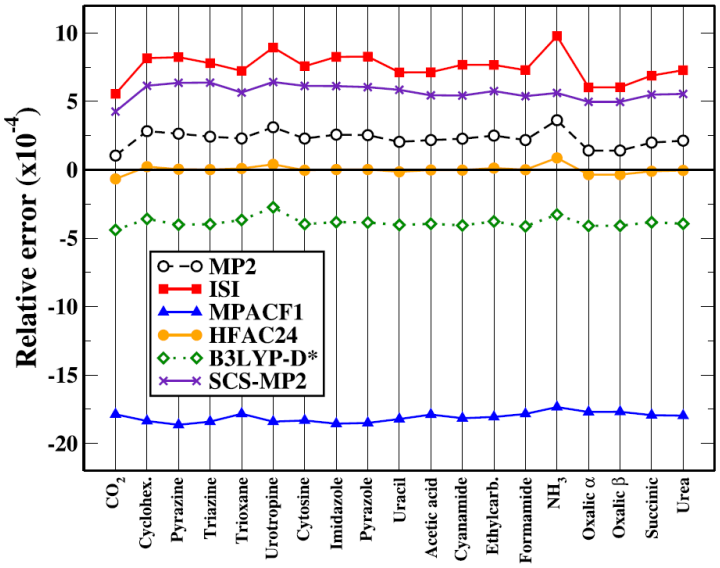
HFAC24 for molecular crystals

System	type	HF	MP2	ISI	revISI	MPACF1	HFAC24
CO_2	disp	25.71	-3.36	0.22	0.29	-0.30	**0.01**
1,4-Cyclohexanedione	disp	89.29	-9.66	5.26	5.90	4.66	**-0.88**
Pyrazine	disp	87.68	-18.74	-0.59	**0.41**	1.33	-8.85
Triazine	disp	74.92	-11.44	**2.59**	3.32	3.17	-3.05
Trioxane	disp	77.30	**-0.61**	11.44	12.04	11.74	7.66
Urotropine	disp	108.92	-16.28	**4.46**	5.50	5.69	-4.52
Cytosine	mixed	119.20	-17.05	5.33	6.61	5.59	**-3.37**
Imidazole	mixed	77.26	-12.83	**2.17**	2.96	3.15	-4.24
Pyrazole	mixed	69.98	-14.94	-0.66	**0.11**	0.46	-6.48
Uracil	mixed	102.71	-15.68	3.21	4.26	**2.92**	-3.33
Acetic acid	H-bond	55.76	**-0.09**	7.46	7.71	6.25	5.49
Cyanamide	H-bond	50.29	-11.03	-1.79	**-1.37**	-2.15	-4.81
Ethylcarbamate	H-bond	74.22	**-2.27**	8.84	9.26	8.44	5.13
Formamide	H-bond	50.89	**-2.03**	5.56	5.85	4.75	3.59
NH_3	H-bond	32.45	**-0.17**	4.39	4.48	4.28	3.22
Oxalic acid α	H-bond	62.56	-5.49	3.66	4.00	**1.81**	2.46
Oxalic acid β	H-bond	66.72	-6.99	3.40	3.87	1.98	**1.74**
Succinic acid	H-bond	106.96	**-1.46**	14.32	15.03	12.80	9.86
Urea	H-bond	55.90	-6.62	2.06	2.37	0.72	**-0.05**
ME		73.09	-8.25	4.28	4.87	4.07	**-0.02**
MAE		73.09	8.25	4.60	5.02	4.33	**4.14**
MARE		86.94%	9.71%	5.49%	5.93%	5.26%	**5.16%**
Std. Dev.		24.73	6.24	3.99	4.00	**3.75**	4.91



High accuracy without error compensation on total energies



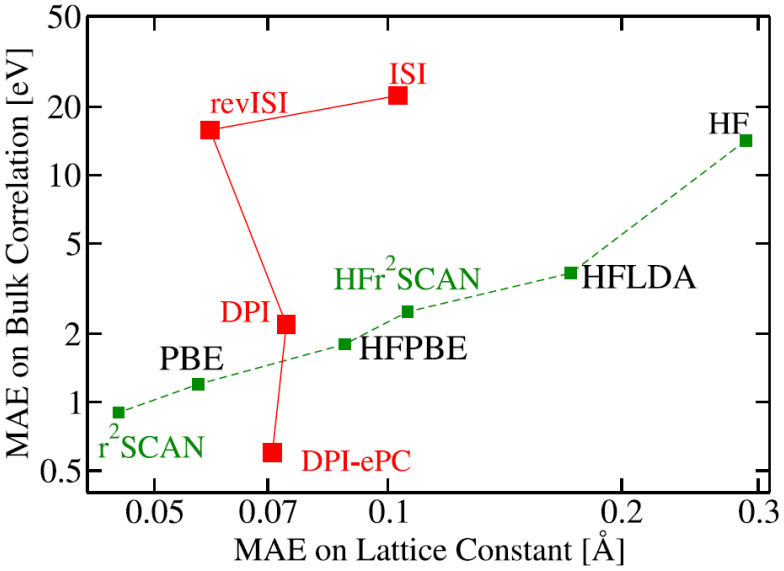
Fabiano, Sarcinella, Della Sala, Ribaldone, Constantin, Dona', Civalleri, Maschio, JCTC 22, 5164 (2026)

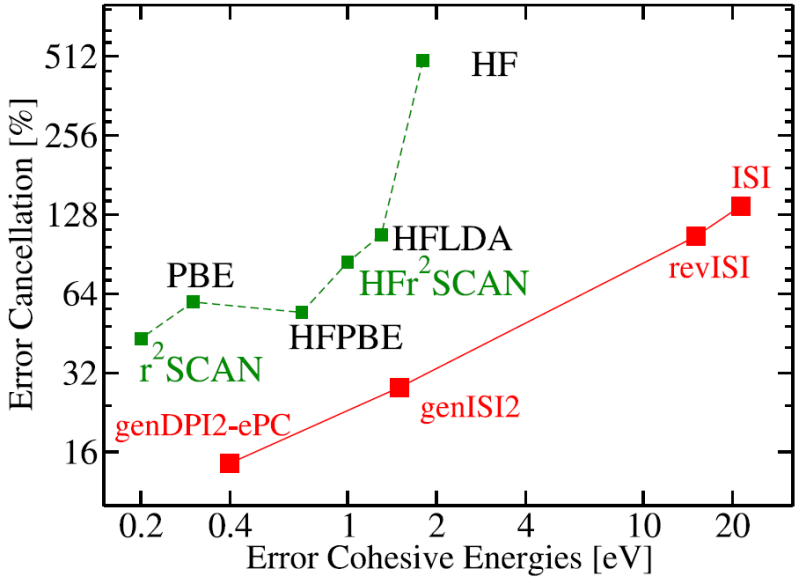
Periodic MP2/CBS calculations with CRYSTAL23

ACII for metallic bulk systems

We also tested ACII methods for metallic solids (Li,Na,K,Al,Cu,Ag,Au)

Della Sala, Sarcinella, Constantin, Dona', Fabiano, Maschio, Civalleri, JCPL 2026 in press





These systems are quite challenging: we used HF ground-state with pseudopotentials (using CRYSTAL23) and a meta-GGA strong interaction functional with the correct Wigner limit (ePC).

Results are comparable to PBE and R2SCAN without any error cancellation !

ePC model:
Constantin, Naeem, Fabiano, Sarcinella, Della Sala, Phys. Rev. B 113, 085121 (2006)

ACM methods in FHI-AIMS

1) To compute the ACM energy, prepare the `control.in` with:

```
xc                  MP2          ──────────►  to compute HF and MP3
total_energy_method HFAC24| hPC | PC  ──►  to compute W,W'
output              rho_on_atoms ──────────►  to compute W3/4
```

2) Run FHI-aims and save the output in aims.out

3) Run the script

acmxc.py -f HFAC24|ISI|revISI|genISI2

```
SCF energy:              -76.0595634400
HF-exchange energy:       -8.9321064100
E_el energy:             -19.2783191263
W_1/2 energy:             74.3220700730
W_{c,inf}^HF energy:     -28.2104255363
W_3/4 energy:            -44.2414675115
MP2 corr. energy:         -0.3261503200
```

NEW: Silicon lattice constant (periodic MP2)

HF	**5.511 (5.512paw)**
MP2	**5.437 (5.415paw)**
HFAC24	**5.425**
REF	**5.416**

```
RESULTS:
 Correlation energy:                  -0.3402448243
 Exchange-correlation energy:         -9.2723512343
 Total energy:                       -76.3998082643
```

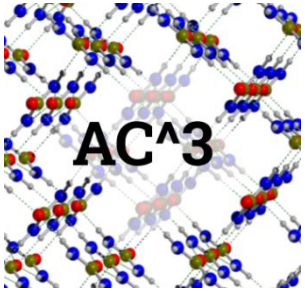
Conclusion

In the last 3 years we made several progresses in the development of Adiabatic Connection Integrand Interpolation methods.

Functionals like HFAC24 or genDPI-ePC are now competitive with state-of-art DFT functionals, and without any error cancellation.

Note that these functionals are non-empirical, i.e. do not include any parameters from real molecular systems, but we considered only atoms and in the strong interaction regime.

Thanks & Collaborators



PRIN project

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