

List of available exchange-correlation functionals in ERKALE

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This is a list of the functionals currently available in the LIBXC trunk, <http://www.tddft.org/programs/octopus/wiki/index.php/Libxc>, which can be used in ERKALE. You can also check the wiki list of the functionals in LIBXC at http://www.tddft.org/programs/octopus/wiki/index.php/Libxc_functionals.

N.B. Some functionals, like ω B97X-D or mBEEF-vdW assume extra contributions that are not implemented in ERKALE. Because LIBXC does not offer a way to check if such further contributions are necessary, it is your responsibility to check that the functional yields correct results.

To run exchange-only or correlation-only calculations in ERKALE, use *none* as the functional, e.g. *none-gga_c_pbe* or *gga_x_pbe-none*. You can also run calculations without any exchange or correlation with *none* or *none-none*. Note that this is not equal to Hartree theory, as the self-interaction term is not removed.

LDA exchange

LDA_X	[1] [2]	Slater exchange
LDA_X_1D	[1]	Exchange in 1D
LDA_X_2D	[1] [2]	Slater exchange

LDA correlation

LDA_C_1D_CSC	[1]	Casula, Sorella & Senatore
LDA_C_1D_LOOS	[1]	P-F Loos correlation LDA
LDA_C_2D_AMGB	[1]	AMGB (for 2D systems)
LDA_C_2D_PRM	[1]	PRM (for 2D systems)
LDA_C_GL	[1]	Gunnarson & Lundqvist
LDA_C_GOMBAS		Gombas
LDA_C_HL	[1]	Hedin & Lundqvist
LDA_C_ML1	[1]	Modified LSD (version 1) of Proynov and Salahub
LDA_C_ML2	[1]	Modified LSD (version 2) of Proynov and Salahub
LDA_C_OB_PW	[1] [2] [3]	Ortiz & Ballone (PW parametrization)
LDA_C_OB_PZ	[1] [2]	Ortiz & Ballone (PZ parametrization)
LDA_C_PW	[1]	Perdew & Wang
LDA_C_PW_MOD	[1]	Perdew & Wang (modified)
LDA_C_PW_RPA	[1]	Perdew & Wang (fit to the RPA energy)
LDA_C_PZ	[1]	Perdew & Zunger
LDA_C_PZ_MOD	[1]	Perdew & Zunger (Modified)
LDA_C_RC04	[1]	Ragot-Cortona
LDA_C_RPA	[1]	Random Phase Approximation (RPA)
LDA_C_VBH	[1]	von Barth & Hedin
LDA_C_VWN	[1]	Vosko, Wilk & Nusair (VWN5)
LDA_C_VWN_1	[1]	Vosko, Wilk & Nusair (VWN1)
LDA_C_VWN_2	[1]	Vosko, Wilk & Nusair (VWN2)
LDA_C_VWN_3	[1]	Vosko, Wilk & Nusair (VWN3)
LDA_C_VWN_4	[1]	Vosko, Wilk & Nusair (VWN4)
LDA_C_VWN_RPA	[1]	Vosko, Wilk & Nusair (VWN5_RPA)
LDA_C_WIGNER	[1]	Wigner
LDA_C_XALPHA	[1]	Slater's Xalpha

LDA exchange-correlation

LDA_XC_KSDT	[1]	Karasiev, Sjostrom, Dufty & Trickey
LDA_XC_TETER93	[1]	Teter 93

LDA_XC_ZLP	[1]	Zhao, Levy & Parr, Eq. (20)
GGA exchange		
GGA_C_PBE_MOL	[1]	Reparametrized PBE by del Campo, Gazquez, Trickey & Vela
GGA_X_2D_B86		Becke 86 in 2D
GGA_X_2D_B86_MGC	[1]	Becke 86 with modified gradient correction for 2D
GGA_X_2D_B88		Becke 88 in 2D
GGA_X_2D_PBE		Perdew, Burke & Ernzerhof in 2D
GGA_X_AIRY	[1]	Constantin et al based on the Airy gas
GGA_X_AK13	[1]	Armiento & Kuemmel 2013
GGA_X_AM05	[1] [2]	Armiento & Mattsson 05
GGA_X_APBE	[1]	mu fixed from the semiclassical neutral atom
GGA_X_B86	[1]	Becke 86
GGA_X_B86_MGC	[1] [2]	Becke 86 with modified gradient correction
GGA_X_B86_R	[1] [2] [3]	Revised Becke 86 with modified gradient correction
GGA_X_B88	[1]	Becke 88
GGA_X_BAYESIAN	[1]	Bayesian best fit for the enhancement factor
GGA_X_BCGP		Burke, Cancio, Gould, and Pittalis
GGA_X_BEEFVDW	[1]	BEEF-vdW exchange
GGA_X_BPCCAC	[1]	BPCCAC (GRAC for the energy)
GGA_X_C09X	[1]	C09x to be used with the VdW of Rutgers-Chalmers
GGA_X_CAP	[1]	Correct Asymptotic Potential
GGA_X_DK87_R1	[1]	dePristo & Kress 87 version R1
GGA_X_DK87_R2	[1]	dePristo & Kress 87 version R2
GGA_X_EB88	[1]	Non-empirical (excogitated) B88 functional of Becke and Elliott
GGA_X_EV93	[1]	Engel and Vosko
GGA_X_FT97_A	[1]	Filatov & Thiel 97 (version A)
GGA_X_FT97_B	[1]	Filatov & Thiel 97 (version B)
GGA_X_G96	[1]	Gill 96
GGA_X_GAM	[1]	GAM functional from Minnesota
GGA_X_HCTH_A	[1]	HCTH-A
GGA_X_HERMAN	[1] [2]	Herman Xalphabeta GGA
GGA_X_HJS_B88	[1]	HJS screened exchange B88 version
GGA_X_HJS_B88_V2	[1]	HJS screened exchange B88 corrected version
GGA_X_HJS_B97X	[1]	HJS screened exchange B97x version
GGA_X_HJS_PBE	[1]	HJS screened exchange PBE version
GGA_X_HJS_PBE_SOL	[1]	HJS screened exchange PBE_SOL version
GGA_X_HTBS	[1]	Haas, Tran, Blaha, and Schwarz
GGA_X_ITYH	[1]	Short-range recipe for exchange GGA functionals
GGA_X_KT1	[1]	Keal and Tozer, version 1
GGA_X_LAG	[1]	Local Airy Gas
GGA_X_LAMBDA_CH_N	[1]	lambda_CH(N) version of PBE
GGA_X_LAMBDA_LO_N	[1]	lambda_LO(N) version of PBE
GGA_X_LAMBDA_OC2_N	[1]	lambda_OC2(N) version of PBE
GGA_X_LB	[1]	van Leeuwen & Baerends
GGA_X_LBM	[1]	van Leeuwen & Baerends modified
GGA_X_LG93	[1]	Lacks & Gordon 93
GGA_X_IV_RPW86	[1]	Berland and Hyldgaard
GGA_X_MB88	[1]	Modified Becke 88 for proton transfer
GGA_X_MPBE	[1]	Adamo & Barone modification to PBE
GGA_X_MPW91	[1]	mPW91 of Adamo & Barone
GGA_X_N12	[1]	Minnesota N12 exchange functional to be used with gga_c_n12
GGA_X_OL2	[1] [2]	Exchange form based on Ou-Yang and Levy v.2
GGA_X_OPTB88_VDW	[1]	opt-Becke 88 for vdW
GGA_X_OPTPBE_VDW	[1]	Reparametrized PBE for vdW
GGA_X_OPTX	[1]	Handy & Cohen OPTX 01
GGA_X_PBE	[1] [2]	Perdew, Burke & Ernzerhof
GGA_X_PBE_JSJR	[1]	Reparametrized PBE by Pedroza, Silva & Capelle

GGA_X_PBE_MOL	[1]	Reparametrized PBE by del Campo, Gazquez, Trickey & Vela
GGA_X_PBE_R	[1]	Revised PBE from Zhang & Yang
GGA_X_PBE_SOL	[1]	Perdew, Burke & Ernzerhof SOL
GGA_X_PBE_TCA	[1]	PBE revised by Tognetti et al
GGA_X_PBEA	[1]	Madsen 07
GGA_X_PBEFE	[1]	PBE for formation energies
GGA_X_PBEINT	[1]	PBE for hybrid interfaces
GGA_X_PBEK1_VDW	[1]	Reparametrized PBE for vdW
GGA_X_PW86	[1]	Perdew & Wang 86
GGA_X_PW91	[2] [3]	Perdew & Wang 91
GGA_X_Q2D	[1]	Chiodo et al
GGA_X_RGE2	[1]	Regularized PBE
GGA_X_RPBE	[1]	Hammer, Hansen, and Norskov
GGA_X_RPW86	[1]	Refitted Perdew & Wang 86
GGA_X_SFAT	[1] [2]	Short-range recipe for exchange GGA functionals - Yukawa
GGA_X_SOGGA	[1]	Second-order generalized gradient approximation
GGA_X_SOGGA11	[1]	Second-order generalized gradient approximation 2011
GGA_X_SSB	[1]	Swarta, Sola and Bickelhaupt
GGA_X_SSB_D	[1]	Swarta, Sola and Bickelhaupt dispersion
GGA_X_SSB_SW	[1]	Swarta, Sola and Bickelhaupt correction to PBE
GGA_X_VMT84_GE	[1]	VMT8,4 with constraint satisfaction with $\mu = \mu_{GE}$
GGA_X_VMT84_PBE	[1]	VMT8,4 with constraint satisfaction with $\mu = \mu_{PBE}$
GGA_X_VMT_GE	[1]	Vela, Medel, and Trickey with $\mu = \mu_{GE}$
GGA_X_VMT_PBE	[1]	Vela, Medel, and Trickey with $\mu = \mu_{PBE}$
GGA_X_WC	[1]	Wu & Cohen
GGA_X_WPBEH	[1] [2] [3] [4] [5]	short-range part of the PBE (default $w=0$ gives PBEh)
GGA_X_XPBE	[1]	Extended PBE by Xu & Goddard III

GGA correlation

GGA_C_AM05	[1] [2]	Armiento & Mattsson 05
GGA_C_APBE	[1]	μ fixed from the semiclassical neutral atom
GGA_C_BCGP		Burke, Cancio, Gould, and Pittalis
GGA_C_BMK	[1]	Boese-Martin for kinetics
GGA_C_FT97	[1] [2]	Filatov & Thiel correlation
GGA_C_GAM	[1]	GAM functional from Minnesota
GGA_C_HCTH_A	[1]	HCTH-A
GGA_C_HYB_TAU_HCTH	[1]	correlation part of hyb-tau-hcth
GGA_C_LM	[1] [2]	Langreth & Mehl
GGA_C_LYP	[1] [2]	Lee, Yang & Parr
GGA_C_N12	[1]	Minnesota N12 functional
GGA_C_N12_SX	[1]	Minnesota N12-SX functional
GGA_C_OP_B88	[1]	one-parameter progressive functional (B88 version)
GGA_C_OP_G96	[1] [2]	one-parameter progressive functional (G96 version)
GGA_C_OP_PBE	[1] [2]	one-parameter progressive functional (PBE version)
GGA_C_OP_PW91	[1] [2]	one-parameter progressive functional (PW91 version)
GGA_C_OP_XALPHA	[1] [2]	one-parameter progressive functional (Xalpha version)
GGA_C_OPTC	[1]	Optimized correlation functional of Cohen and Handy
GGA_C_P86	[1]	Perdew 86
GGA_C_PBE	[1] [2]	Perdew, Burke & Ernzerhof
GGA_C_PBE_JRGX	[1]	Reparametrized PBE by Pedroza, Silva & Capelle
GGA_C_PBE_SOL	[1]	Perdew, Burke & Ernzerhof SOL
GGA_C_PBEFE	[1]	PBE for formation energies
GGA_C_PBEINT	[1]	PBE for hybrid interfaces
GGA_C_PBELOC	[1]	Semilocal dynamical correlation
GGA_C_PW91	[2] [3]	Perdew & Wang 91
GGA_C_Q2D	[1]	Chiodo et al
GGA_C_REGTPSS	[1]	regularized TPSS correlation
GGA_C_REVTCA	[1]	Tognetti, Cortona, Adamo (revised)

GGA_C_RGE2	[1]	Regularized PBE
GGA_C_SOGGA11	[1]	Second-order generalized gradient approximation 2011
GGA_C_SOGGA11_X	[1]	To be used with HYB_GGA_X_SOGGA11_X
GGA_C_SPBE	[1]	PBE correlation to be used with the SSB exchange
GGA_C_TAU_HCTH	[1]	correlation part of tau-hcth
GGA_C_TCA	[1]	Tognetti, Cortona, Adamo
GGA_C_WI	[1]	Wilson & Ivanov
GGA_C_WI0	[1]	Wilson & Ivanov initial version
GGA_C_WL	[1]	Wilson & Levy
GGA_C_XPBE	[1]	Extended PBE by Xu & Goddard III
GGA_C_ZPBEINT	[1]	spin-dependent gradient correction to PBEint
GGA_C_ZPBESOL	[1]	spin-dependent gradient correction to PBEsol

GGA exchange-correlation

GGA_XC_B97_D	[1]	Becke 97-D
GGA_XC_B97_GGA1	[1]	Becke 97 GGA-1
GGA_XC_BEEFVDW	[1]	BEEF-vdW exchange-correlation
GGA_XC_EDF1	[1]	EDF1
GGA_XC_HCTH_120	[1]	HCTH/120
GGA_XC_HCTH_147	[1]	HCTH/147
GGA_XC_HCTH_407	[1]	HCTH/407
GGA_XC_HCTH_407P	[1]	HCTH/407+
GGA_XC_HCTH_93	[1]	HCTH/93
GGA_XC_HCTH_P14	[1]	HCTH p=1/4
GGA_XC_HCTH_P76	[1]	HCTH p=7/6
GGA_XC_KT2	[1]	Keal and Tozer, version 2
GGA_XC_MOHLYP	[1]	Functional for organometallic chemistry
GGA_XC_MOHLYP2	[1]	Functional for barrier heights
GGA_XC_MPWLYP1W	[1]	mPWLYP1w
GGA_XC_OBLYP_D	[1]	oBLYP-D functional of Goerigk and Grimme
GGA_XC_OPBE_D	[1]	oPBE-D functional of Goerigk and Grimme
GGA_XC_OPWLYP_D	[1]	oPWLYP-D functional of Goerigk and Grimme
GGA_XC_PBE1W	[1]	PBE1W
GGA_XC_PBELYP1W	[1]	PBELYP1W
GGA_XC_TH1	[1]	Tozer and Handy v. 1
GGA_XC_TH2	[1]	Tozer and Handy v. 2
GGA_XC_TH3	[1]	Tozer and Handy v. 3
GGA_XC_TH4	[1]	Tozer and Handy v. 4
GGA_XC_TH_FC	[1]	Tozer and Handy v. FC
GGA_XC_TH_FCFO	[1]	Tozer and Handy v. FCFO
GGA_XC_TH_FCO	[1]	Tozer and Handy v. FCO
GGA_XC_TH_FL	[1]	Tozer and Handy v. FL
GGA_XC_VV10	[1]	Vydrov and Van Voorhis
GGA_XC_XLYP	[1]	XLYP

hybrid GGA exchange

HYB_GGA_X_N12_SX	[1]	Worker for hyb_gga_x_n12_sx
HYB_GGA_X_SOGGA11_X	[1]	Hybrid based on SOGGA11 form

hybrid GGA exchange-correlation

HYB_GGA_XC_B1LYP	[1]	B1LYP
HYB_GGA_XC_B1PW91	[1]	B1PW91
HYB_GGA_XC_B1WC	[1]	B1WC
HYB_GGA_XC_B3LYP	[1]	B3LYP
HYB_GGA_XC_B3LYP5	[1]	B3LYP with VWN functional 5 instead of RPA
HYB_GGA_XC_B3LYPS	[1]	B3LYP*
HYB_GGA_XC_B3P86	[1]	B3P86

HYB_GGA_XC_B3PW91	[1]	The original (ACM, B3PW91) hybrid of Becke
HYB_GGA_XC_B97	[1]	Becke 97
HYB_GGA_XC_B97_1	[1]	Becke 97-1
HYB_GGA_XC_B97_1P	[1]	version of B97 by Cohen and Handy
HYB_GGA_XC_B97_2	[1]	Becke 97-2
HYB_GGA_XC_B97_3	[1]	Becke 97-3
HYB_GGA_XC_B97_K	[1]	Boese-Martin for Kinetics
HYB_GGA_XC_BHANDH	[1]	BHandH
HYB_GGA_XC_BHANDHLYP	[1]	BHandHLYP
HYB_GGA_XC_CAM_B3LYP	[1]	CAM version of B3LYP
HYB_GGA_XC_CAMY_B3LYP	[1]	CAMY version of B3LYP
HYB_GGA_XC_CAMY_BLYP	[1]	CAMY version of BLYP
HYB_GGA_XC_CAO0	[1]	Correct Asymptotic Potential hybrid
HYB_GGA_XC_EDF2	[1]	EDF2
HYB_GGA_XC_HJS_B88	[1]	HJS hybrid screened exchange B88 version
HYB_GGA_XC_HJS_B97X	[1]	HJS hybrid screened exchange B97x version
HYB_GGA_XC_HJS_PBE	[1]	HJS hybrid screened exchange PBE version
HYB_GGA_XC_HJS_PBE_SOL	[1]	HJS hybrid screened exchange PBE_SOL version
HYB_GGA_XC_HPBEINT	[1]	hPBEint
HYB_GGA_XC_HSE03	[1] [2]	HSE03
HYB_GGA_XC_HSE06	[1] [2] [3]	HSE06
HYB_GGA_XC_HSE12	[1]	HSE12
HYB_GGA_XC_HSE12S	[1]	HSE12 (short-range version)
HYB_GGA_XC_HSE_SOL	[1]	HSEsol
HYB_GGA_XC_LC_VV10	[1]	Vydrov and Van Voorhis
HYB_GGA_XC_LC_WPBE	[1]	Long-range corrected PBE (LC-wPBE) by Vydrov and Scuseria
HYB_GGA_XC_LCY_BLYP	[1] [2]	LCY version of BLYP
HYB_GGA_XC_LCY_PBE	[1] [2]	LCY version of PBE
HYB_GGA_XC_LRC_WPBE	[1]	Long-range corrected PBE (LRC-wPBE) by Rohrdanz, Martins and He
HYB_GGA_XC_LRC_WPBEH	[1]	Long-range corrected short-range hybrid PBE (LRC-wPBEh) by Rohrd
HYB_GGA_XC_MB3LYP_RC04	[1]	B3LYP with RC04 LDA
HYB_GGA_XC_MPW1K	[1]	mPW1K
HYB_GGA_XC_MPW1PW	[1]	mPW1PW
HYB_GGA_XC_MPW3LYP	[1]	MPW3LYP
HYB_GGA_XC_MPW3PW	[1]	MPW3PW of Adamo & Barone
HYB_GGA_XC_MPWLYP1M	[1]	MPW with 1 par. for metals/LYP
HYB_GGA_XC_O3LYP	[1]	O3LYP
HYB_GGA_XC_PBE0_13	[1]	PBE0-1/3
HYB_GGA_XC_PBE_MOL0	[1]	PBEsol0
HYB_GGA_XC_PBE_MOLB0	[1]	PBEsolbeta0
HYB_GGA_XC_PBE_SOLO	[1]	PBEsol0
HYB_GGA_XC_PBEB0	[1]	PBEbeta0
HYB_GGA_XC_PBEH	[1] [2]	PBEH (PBE0)
HYB_GGA_XC_REVB3LYP	[1]	Revised B3LYP
HYB_GGA_XC_SB98_1A	[1]	SB98 (1a)
HYB_GGA_XC_SB98_1B	[1]	SB98 (1b)
HYB_GGA_XC_SB98_1C	[1]	SB98 (1c)
HYB_GGA_XC_SB98_2A	[1]	SB98 (2a)
HYB_GGA_XC_SB98_2B	[1]	SB98 (2b)
HYB_GGA_XC_SB98_2C	[1]	SB98 (2c)
HYB_GGA_XC_TUNED_CAM_B3LYP	[1]	CAM version of B3LYP, tuned for excitations and properties
HYB_GGA_XC_WB97	[1]	wB97 range-separated functional
HYB_GGA_XC_WB97X	[1]	wB97X range-separated functional
HYB_GGA_XC_WB97X_D	[1]	wB97D range-separated functional
HYB_GGA_XC_WB97X_V	[1]	wB97X-V range-separated functional
HYB_GGA_XC_X3LYP	[1]	X3LYP

meta-GGA exchange

HYB_MGGA_X_M06_2X	[1]	M06-2X functional from Minnesota
MGGA_X_2D_PRHG07	[1]	Pittalis-Rasanen-Helbig-Gross 2007
MGGA_X_2D_PRHG07_PRP10	[1] [2]	PRHG07 with Pittalis-Rasanen-Proetto 2010 correction
MGGA_X_B00	[1]	Becke 2000
MGGA_X_BJ06	[1]	Becke & Johnson 06
MGGA_X_BLOC	[1]	functional with balanced localization
MGGA_X_BMK	[1]	Boese-Martin for kinetics
MGGA_X_BR89	[1]	Becke-Roussel 89
MGGA_X_GVT4	[1]	GVT4 (X part of VSXC)
MGGA_X_LTA	[1]	Local tau approximation
MGGA_X_M06	[1]	Worker for hyb_mgga_xc_m06
MGGA_X_M06_HF	[1]	Worker for hyb_mgga_xc_m06_hf
MGGA_X_M06_L	[1] [2]	Minnesota M06-L functional
MGGA_X_M08_HX	[1]	Worker for hyb_mgga_x_m08_hx
MGGA_X_M08_SO	[1]	Worker for hyb_mgga_x_m08_so
MGGA_X_M11	[1]	Worker for hyb_mgga_xc_m11
MGGA_X_M11_L	[1]	Minnesota M11-L exchange functional
MGGA_X_MBEEF	[1]	mBEEF exchange
MGGA_X_MBEEFVDW		mBEEF-vdW exchange
MGGA_X_MK00	[1]	Exchange for accurate virtual orbital energies
MGGA_X_MK00B	[1]	Exchange for accurate virtual orbital energies (v. B)
MGGA_X_MN12_L	[1]	Minnesota MN12-L functional
MGGA_X_MN15_L	[1]	Minnesota MN15-L functional
MGGA_X_MODTPSS	[1]	Modified Tao, Perdew, Staroverov & Scuseria
MGGA_X_MS0	[1]	MS exchange of Sun, Xiao, and Ruzsinszky
MGGA_X_MS1	[1]	MS1 exchange of Sun, et al
MGGA_X_MS2	[1]	MS2 exchange of Sun, et al
MGGA_X_MVS	[1]	MVS exchange of Sun, Perdew, and Ruzsinszky
MGGA_X_PKZB	[1]	Perdew, Kurth, Zupan, and Blaha
MGGA_X_REVTPSS	[1] [2]	revised Tao, Perdew, Staroverov & Scuseria
MGGA_X_RPP09	[1]	Rasanen, Pittalis & Proetto 09
MGGA_X_SCAN	[1]	SCAN exchange of Sun, Ruzsinszky, and Perdew
MGGA_X_TAU_HCTH	[1]	tau-HCTH from Boese and Handy
MGGA_X_TB09	[1]	Tran & Blaha 09
MGGA_X_TPSS	[1] [2]	Tao, Perdew, Staroverov & Scuseria

meta-GGA correlation

MGGA_C_BC95	[1]	Becke correlation 95
MGGA_C_CS	[1]	Colle and Salvetti
MGGA_C_DLDF	[1]	Dispersionless Density Functional
MGGA_C_M05	[1]	Worker for hyb_mgga_xc_m05
MGGA_C_M05_2X	[1]	Worker for hyb_mgga_xc_m05_2x
MGGA_C_M06	[1]	Worker for hyb_mgga_xc_m06
MGGA_C_M06_2X	[1]	Worker for hyb_mgga_xc_m06_2x
MGGA_C_M06_HF	[1]	Worker for hyb_mgga_xc_m06_hf
MGGA_C_M06_L	[1] [2]	Minnesota M06-L functional
MGGA_C_M08_HX	[1]	Worker for hyb_mgga_xc_m08_hx
MGGA_C_M08_SO	[1]	Worker for hyb_mgga_xc_m08_so
MGGA_C_M11	[1]	Worker for hyb_mgga_xc_m11
MGGA_C_M11_L	[1]	Minnesota M11-L correlation functional
MGGA_C_MN12_L	[1]	Minnesota MN12-L correlation functional
MGGA_C_MN12_SX	[1]	Worker for hyb_mgga_xc_mn12_sx
MGGA_C_MN15	[1]	Minnesota MN15 correlation functional
MGGA_C_MN15_L	[1]	Minnesota MN15-L correlation functional
MGGA_C_PKZB	[1]	Perdew, Kurth, Zupan, and Blaha
MGGA_C_REVTPSS	[1] [2]	revised TPSS correlation
MGGA_C_SCAN	[1]	SCAN correlation of Sun, Ruzsinszky, and Perdew
MGGA_C_TPSS	[1] [2]	Tao, Perdew, Staroverov & Scuseria

MGGA_C_TPSSLOC	[1]	Semilocal dynamical correlation
MGGA_C_VSXC	[1]	VSXC (correlation part)
meta-GGA exchange-correlation		
MGGA_XC_B97M_V	[1]	B97M-V exchange-correlation functional
MGGA_XC_CC06	[1]	Cancio and Chou 2006
MGGA_XC_OTPSS_D	[1]	oTPSS-D functional of Goerigk and Grimme
MGGA_XC_TPSSLYP1W	[1]	TPSSLYP1W
MGGA_XC_ZLP	[1]	Zhao, Levy & Parr, Eq. (21)
hybrid meta-GGA exchange		
HYB_MGGA_X_DLDF	[1]	Dispersionless Density Functional
HYB_MGGA_X_M05	[1]	Minnesota M05 functional
HYB_MGGA_X_M05_2X	[1]	M05-2X functional from Minnesota
HYB_MGGA_X_MN12_SX	[1]	Minnesota MN12-SX hybrid functional
HYB_MGGA_X_MN15	[1]	Minnesota MN15 hybrid functional
HYB_MGGA_X_MS2H	[1]	MS2 hybrid exchange of Sun, et al
HYB_MGGA_X_MVSH	[1]	MVSh hybrid exchange functional
HYB_MGGA_X_SCAN0	[1]	SCAN hybrid exchange (SCAN0)
HYB_MGGA_X_TAU_HCTH	[1]	Hybrid version of tau-HCTH
hybrid meta-GGA exchange-correlation		
HYB_MGGA_XC_B86B95	[1]	Mixture of B86 with BC95
HYB_MGGA_XC_B88B95	[1]	Mixture of B88 with BC95 (B1B95)
HYB_MGGA_XC_BB1K	[1]	Mixture of B88 with BC95 from Zhao and Truhlar
HYB_MGGA_XC_M06	[1]	Minnesota M06 functional
HYB_MGGA_XC_M06_HF	[1]	Minnesota M06-HF functional
HYB_MGGA_XC_M08_HX	[1]	Minnesota M08-HX hybrid functional
HYB_MGGA_XC_M08_SO	[1]	Minnesota M08-SO hybrid functional
HYB_MGGA_XC_M11	[1]	Minnesota M11 hybrid functional
HYB_MGGA_XC_MPW1B95	[1]	Mixture of mPW91 with BC95 from Zhao and Truhlar
HYB_MGGA_XC_MPWB1K	[1]	Mixture of mPW91 with BC95 for kinetics
HYB_MGGA_XC_PW6B95	[1]	Mixture of PW91 with BC95 from Zhao and Truhlar
HYB_MGGA_XC_PW86B95	[1]	Mixture of PW86 with BC95
HYB_MGGA_XC_PWB6K	[1]	Mixture of PW91 with BC95 from Zhao and Truhlar for kinetics
HYB_MGGA_XC_REVTPSSH	[1]	revTPSSh
HYB_MGGA_XC_TPSSH	[1]	TPSSh
HYB_MGGA_XC_WB97M_V	[1]	wB97M-V exchange-correlation functional
HYB_MGGA_XC_X1B95	[1]	Mixture of X with BC95
HYB_MGGA_XC_XB1K	[1]	Mixture of X with BC95 for kinetics