

## 4.5 brian\_macros\_functionals.h File Reference

### Macros

#### DFT functional IDs

- #define BRIAN\_FUNCTIONAL\_EXACT\_EXCHANGE 1010000000UL  
*Exact Hartree-Fock exchange.*
- #define BRIAN\_FUNCTIONAL\_EXACT\_EXCHANGE\_SHORT\_RANGE 1010000001UL  
*Short-range component of the Hartree-Fock exact exchange.*
- #define BRIAN\_FUNCTIONAL\_EXACT\_EXCHANGE\_LONG\_RANGE 1010000002UL  
*Long-range component of the Hartree-Fock exact exchange.*
- #define BRIAN\_FUNCTIONAL\_GGA\_AIRY\_X 1010000003UL  
*Constantin et al based on the Airy gas*  
*References:*  
*L. A. Constantin, A. Ruzsinszky, and J. P. Perdew, Phys. Rev. B 80, 035125 (2009) (10.1103/PhysRevB.80.035125)*
- #define BRIAN\_FUNCTIONAL\_GGA\_AK13\_X 1010000004UL  
*Armiento & Kuemmel 2013*  
*References:*  
*R. Armiento and S. Kümmel, Phys. Rev. Lett. 111, 036402 (2013) (10.1103/PhysRevLett.111.036402)*
- #define BRIAN\_FUNCTIONAL\_GGA\_AM05\_C 1010000005UL  
*Armiento & Mattsson 05*  
*References:*  
*R. Armiento and A. E. Mattsson, Phys. Rev. B 72, 085108 (2005) (10.1103/PhysRevB.72.085108)*  
*A. E. Mattsson, R. Armiento, J. Paier, G. Kresse, J. M. Wills, and T. R. Mattsson, J. Chem. Phys. 128, 084714 (2008) (10.1063/1.2835596)*
- #define BRIAN\_FUNCTIONAL\_GGA\_AM05\_X 1010000006UL  
*Armiento & Mattsson 05*  
*References:*  
*R. Armiento and A. E. Mattsson, Phys. Rev. B 72, 085108 (2005) (10.1103/PhysRevB.72.085108)*  
*A. E. Mattsson, R. Armiento, J. Paier, G. Kresse, J. M. Wills, and T. R. Mattsson, J. Chem. Phys. 128, 084714 (2008) (10.1063/1.2835596)*
- #define BRIAN\_FUNCTIONAL\_GGA\_APBE\_C 1010000007UL  
*mu fixed from the semiclassical neutral atom*  
*References:*  
*L. A. Constantin, E. Fabiano, S. Laricchia, and F. Della Sala, Phys. Rev. Lett. 106, 186406 (2011) (10.1103/PhysRevLett.106.186406)*
- #define BRIAN\_FUNCTIONAL\_GGA\_APBE\_X 1010000008UL  
*mu fixed from the semiclassical neutral atom*  
*References:*  
*L. A. Constantin, E. Fabiano, S. Laricchia, and F. Della Sala, Phys. Rev. Lett. 106, 186406 (2011) (10.1103/PhysRevLett.106.186406)*
- #define BRIAN\_FUNCTIONAL\_GGA\_B86\_MGC\_X 1010000009UL  
*Becke 86 with modified gradient correction*  
*References:*  
*A. D. Becke, J. Chem. Phys. 84, 4524 (1986) (10.1063/1.450025)*  
*A. D. Becke, J. Chem. Phys. 85, 7184 (1986) (10.1063/1.451353)*
- #define BRIAN\_FUNCTIONAL\_GGA\_B86\_R\_X 1010000010UL  
*Revised Becke 86 with modified gradient correction*  
*References:*  
*I. Hamada, Phys. Rev. B 89, 121103 (2014) (10.1103/PhysRevB.89.121103)*  
*A. D. Becke, J. Chem. Phys. 84, 4524 (1986) (10.1063/1.450025)*  
*A. D. Becke, J. Chem. Phys. 85, 7184 (1986) (10.1063/1.451353)*
- #define BRIAN\_FUNCTIONAL\_GGA\_B86\_X 1010000011UL  
*Becke 86*  
*References:*  
*A. D. Becke, J. Chem. Phys. 84, 4524 (1986) (10.1063/1.450025)*
- #define BRIAN\_FUNCTIONAL\_GGA\_B88M\_X 1010000012UL

- Becke 88 reoptimized to be used with tau1*  
 References:  
 E. Proynov, H. Chermette, and D. R. Salahub, *J. Chem. Phys.* 113, 10013 (2000) (10.1063/1.1321309)
- #define BRIAN\_FUNCTIONAL\_GGA\_B88\_X 1010000013UL  
*Becke 88*  
 References:  
 A. D. Becke, *Phys. Rev. A* 38, 3098 (1988) (10.1103/PhysRevA.38.3098)
  - #define BRIAN\_FUNCTIONAL\_GGA\_B97\_D3\_XC 1010000014UL  
*Becke 97-D*  
 References:  
 S. Grimme, *J. Comput. Chem.* 27, 1787 (2006) (10.1002/jcc.20495)
  - #define BRIAN\_FUNCTIONAL\_GGA\_B97\_D\_XC 1010000015UL  
*Becke 97-D*  
 References:  
 S. Grimme, *J. Comput. Chem.* 27, 1787 (2006) (10.1002/jcc.20495)
  - #define BRIAN\_FUNCTIONAL\_GGA\_B97\_GGA1\_XC 1010000016UL  
*Becke 97 GGA-1*  
 References:  
 A. J. Cohen and N. C. Handy, *Chem. Phys. Lett.* 316, 160 (2000) (10.1016/S0009-2614(99)01273-7)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BAYESIAN\_X 1010000017UL  
*Bayesian best fit for the enhancement factor*  
 References:  
 J. J. Mortensen, K. Kaasbjerg, S. L. Frederiksen, J. K. Nørskov, J. P. Sethna, and K. W. Jacobsen, *Phys. Rev. Lett.* 95, 216401 (2005) (10.1103/PhysRevLett.95.216401)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BCGP\_C 1010000018UL  
*Burke, Cancio, Gould, and Pittalis*  
 References:  
 K. Burke, A. Cancio, T. Gould, and S. Pittalis, *ArXiv e-prints* (2014), arXiv:1409.4834 [cond-mat.mtrl-sci].
  - #define BRIAN\_FUNCTIONAL\_GGA\_BCGP\_X 1010000019UL  
*Burke, Cancio, Gould, and Pittalis*  
 References:  
 K. Burke, A. Cancio, T. Gould, and S. Pittalis, *ArXiv e-prints* (2014), arXiv:1409.4834 [cond-mat.mtrl-sci].
  - #define BRIAN\_FUNCTIONAL\_GGA\_BEEFVDW\_X 1010000020UL  
*BEEF-vdW exchange*  
 References:  
 J. Wellendorff, K. T. Lundgaard, A. M[gelh[j], V. Petzold, D. D. Landis, J. K. N[rskov], T. Bligaard, and K. W. Jacobsen, *Phys. Rev. B* 85, 235149 (2012) (10.1103/PhysRevB.85.235149)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BEEFVDW\_XC 1010000021UL  
*BEEF-vdW exchange-correlation*  
 References:  
 J. Wellendorff, K. T. Lundgaard, A. M[gelh[j], V. Petzold, D. D. Landis, J. K. N[rskov], T. Bligaard, and K. W. Jacobsen, *Phys. Rev. B* 85, 235149 (2012) (10.1103/PhysRevB.85.235149)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BLYP\_XC 1010000022UL  
*B88 exchange and LYP correlation*  
 Functional components: GGA\_B88\_X + GGA\_LYP\_C  
 References:  
 A. D. Becke, *Phys. Rev. A* 38, 3098 (1988) (10.1103/PhysRevA.38.3098)  
 C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B* 37, 785 (1988) (10.1103/PhysRevB.37.785)  
 B. Miehlich, A. Savin, H. Stoll, and H. Preuss, *Chem. Phys. Lett.* 157, 200 (1989) (10.1016/0009-2614(89)87234-3)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BMK\_C 1010000023UL  
*Boese-Martin for kinetics*  
 References:  
 A. D. Boese and J. M. L. Martin, *J. Chem. Phys.* 121, 3405 (2004) (10.1063/1.1774975)
  - #define BRIAN\_FUNCTIONAL\_GGA\_BPCCAC\_X 1010000024UL  
*BPCCAC (GRAC for the energy)*  
 References:  
 E. Br'emond, D. Pilard, I. Ciofini, H. Chermette, C. Adamo, and P. Cortona, *Theor. Chem. Acc.* 131, 1184 (2012) (10.1007/s00214-012-1184-0)
  - #define BRIAN\_FUNCTIONAL\_GGA\_C09X\_X 1010000025UL  
*C09x to be used with the VdW of Rutgers-Chalmers*  
 References:  
 V. R. Cooper, *Phys. Rev. B* 81, 161104 (2010) (10.1103/PhysRevB.81.161104)

- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_CAP\\_X](#) 1010000026UL  
*Correct Asymptotic Potential*  
References:  
*J. Carmona-Espindola, J. L. G'azquez, A. Vela, and S. B. Trickey, J. Chem. Phys. 142, 054105 (2015), 10.1063/1.4906606 (10.1063/1.4906606)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_CHACHIYO\\_X](#) 1010000027UL  
*Chachiyo exchange*  
References:  
*T. {Chachiyo and H. {Chachiyo}, }ArXiv e-prints (2017), arXiv:1706.01343 [cond-mat.mtrl-sci].*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_CS1\\_C](#) 1010000028UL  
*A dynamical correlation functional*  
References:  
*N. C. Handy and A. J. Cohen, J. Chem. Phys. 116, 5411 (2002) (10.1063/1.1457432)*  
*E. I. Proynov and A. J. Thakkar, Int. J. Quantum Chem. 106, 436 (2006) (10.1002/qua.20758)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_DK87\\_R1\\_X](#) 1010000029UL  
*dePristo & Kress 87 version R1*  
References:  
*A. E. DePristo and J. D. Kress, J. Chem. Phys. 86, 1425 (1987) (10.1063/1.452230)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_DK87\\_R2\\_X](#) 1010000030UL  
*dePristo & Kress 87 version R2*  
References:  
*A. E. DePristo and J. D. Kress, J. Chem. Phys. 86, 1425 (1987) (10.1063/1.452230)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_EB88\\_X](#) 1010000031UL  
*Non-empirical (excogitated) B88 functional of Becke and Elliott*  
References:  
*P. Elliott and K. Burke, Can. J. Chem. 87, 1485 (2009) (10.1139/V09-095)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_EDF1\\_XC](#) 1010000032UL  
*EDF1*  
References:  
*R. D. Adamson, P. M. W. Gill, and J. A. Pople, Chem. Phys. Lett. 284, 6 (1998) (10.1016/S0009-2614(97)01282-7)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_EV93\\_X](#) 1010000033UL  
*Engel and Vosko*  
References:  
*E. Engel and S. H. Vosko, Phys. Rev. B 47, 13164 (1993) (10.1103/PhysRevB.47.13164)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_FT97\\_A\\_X](#) 1010000034UL  
*Filatov & Thiel 97 (version A)*  
References:  
*M. Filatov and W. Thiel, Mol. Phys. 91, 847 (1997) (10.1080/002689797170950)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_FT97\\_B\\_X](#) 1010000035UL  
*Filatov & Thiel 97 (version B)*  
References:  
*M. Filatov and W. Thiel, Mol. Phys. 91, 847 (1997) (10.1080/002689797170950)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_FT97\\_C](#) 1010000036UL  
*Filatov & Thiel correlation*  
References:  
*M. Filatov and W. Thiel, Int. J. Quantum Chem. 62, 603 (1997) (10.1002/(SICI)1097-461X(1997)62:6<603::AID-QUA4>3.0.CO;2-#)*  
*M. Filatov and W. Thiel, Mol. Phys. 91, 847 (1997) (10.1080/002689797170950)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_G96\\_X](#) 1010000037UL  
*Gill 96*  
References:  
*P. M. W. Gill, Mol. Phys. 89, 433 (1996) (10.1080/002689796173813)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_GAM\\_X](#) 1010000038UL  
*Minnesota GAM exchange functional*  
References:  
*H. S. Yu, W. Zhang, P. Verma, X. He, and D. G. Truhlar, Phys. Chem. Chem. Phys. 17, 12146 (2015) (10.1039/C5CP01425E)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_GAPC\\_C](#) 1010000039UL  
*GapC*  
References:  
*E. Fabiano, P. E. Trevisanutto, A. Terentjevs, and L. A. Constantin, J. Chem. Theory Comput. 10, 2016 (2014), pMID: 26580528 (10.1021/ct500073b)*

- #define BRIAN\_FUNCTIONAL\_GGA\_GAPLOC\_C 1010000040UL  
     Gaploc  
     References:  
     E. Fabiano, P. E. Trevisanutto, A. Terentjevs, and L. A. Constantin, *J. Chem. Theory Comput.* 10, 2016 (2014),  
     pMID: 26580528 (10.1021/ct500073b)
- #define BRIAN\_FUNCTIONAL\_GGA\_GG99\_X 1010000041UL  
     Gilbert and Gill 1999  
     References:  
     A. T. Gilbert and P. M. Gill, *Chem. Phys. Lett.* 312, 511 (1999) (10.1016/S0009-2614(99)00836-2)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_120\_XC 1010000042UL  
     HCTH/120  
     References:  
     A. D. Boese, N. L. Doltsinis, N. C. Handy, and M. Sprik, *J. Chem. Phys.* 112, 1670 (2000) (10.1063/1.480732)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_147\_XC 1010000043UL  
     HCTH/147  
     References:  
     A. D. Boese, N. L. Doltsinis, N. C. Handy, and M. Sprik, *J. Chem. Phys.* 112, 1670 (2000) (10.1063/1.480732)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_407P\_XC 1010000044UL  
     HCTH/407+  
     References:  
     A. D. Boese, A. Chandra, J. M. L. Martin, and D. Marx, *J. Chem. Phys.* 119, 5965 (2003) (10.1063/1.1599338)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_407\_XC 1010000045UL  
     HCTH/407  
     References:  
     A. D. Boese and N. C. Handy, *J. Chem. Phys.* 114, 5497 (2001) (10.1063/1.1347371)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_93\_XC 1010000046UL  
     HCTH/93  
     References:  
     F. A. Hamprecht, A. J. Cohen, D. J. Tozer, and N. C. Handy, *J. Chem. Phys.* 109, 6264 (1998) (10.1063/1.477267)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_A\_C 1010000047UL  
     HCTH-A  
     References:  
     F. A. Hamprecht, A. J. Cohen, D. J. Tozer, and N. C. Handy, *J. Chem. Phys.* 109, 6264 (1998) (10.1063/1.477267)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_A\_X 1010000048UL  
     HCTH-A  
     References:  
     F. A. Hamprecht, A. J. Cohen, D. J. Tozer, and N. C. Handy, *J. Chem. Phys.* 109, 6264 (1998) (10.1063/1.477267)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_P14\_XC 1010000049UL  
     HCTH p=1/4  
     References:  
     G. Menconi, P. J. Wilson, and D. J. Tozer, *J. Chem. Phys.* 114, 3958 (2001) (10.1063/1.1342776)
- #define BRIAN\_FUNCTIONAL\_GGA\_HCTH\_P76\_XC 1010000050UL  
     HCTH p=7/6  
     References:  
     G. Menconi, P. J. Wilson, and D. J. Tozer, *J. Chem. Phys.* 114, 3958 (2001) (10.1063/1.1342776)
- #define BRIAN\_FUNCTIONAL\_GGA\_HERMAN\_X 1010000051UL  
     Herman Xalphabeta GGA  
     References:  
     F. Herman, J. P. V. Dyke, and I. B. Ortenburger, *Phys. Rev. Lett.* 22, 807 (1969) (10.1103/PhysRevLett.22.807)  
     F. Herman, I. B. Ortenburger, and J. P. V. Dyke, *Int. J. Quantum Chem.* 4, 827 (1969) (10.1002/qua.560040746)
- #define BRIAN\_FUNCTIONAL\_GGA\_HJS\_B88\_V2\_X 1010000052UL  
     HJS screened exchange B88 corrected version  
     References:  
     E. Weintraub, T. M. Henderson, and G. E. Scuseria, *J. Chem. Theory Comput.* 5, 754 (2009) (10.1021/ct800530u)
- #define BRIAN\_FUNCTIONAL\_GGA\_HJS\_B88\_X 1010000053UL  
     HJS screened exchange B88 version  
     References:  
     T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)
- #define BRIAN\_FUNCTIONAL\_GGA\_HJS\_B97X\_X 1010000054UL  
     HJS screened exchange B97x version  
     References:  
     T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)

- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_HJS\\_PBE\\_SOL\\_X](#) 1010000055UL  
*HJS screened exchange PBE\_SOL version*  
References:  
*T. M. Henderson, B. G. Janesko, and G. E. Scuseria, J. Chem. Phys. 128, 194105 (2008) (10.1063/1.2921797)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_HJS\\_PBE\\_X](#) 1010000056UL  
*HJS screened exchange PBE version*  
References:  
*T. M. Henderson, B. G. Janesko, and G. E. Scuseria, J. Chem. Phys. 128, 194105 (2008) (10.1063/1.2921797)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_HLE16\\_XC](#) 1010000057UL  
*high local exchange 2016*  
References:  
*P. Verma and D. G. Truhlar, J. Phys. Chem. Lett. 8, 380 (2017), PMID: 28033712 (10.1021/acs.jpcclett.6b02757)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_HTBS\\_X](#) 1010000058UL  
*Haas, Tran, Blaha, and Schwarz*  
References:  
*P. Haas, F. Tran, P. Blaha, and K. Schwarz, Phys. Rev. B 83, 205117 (2011) (10.1103/PhysRevB.83.205117)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_HYB\\_TAU\\_HCTH\\_C](#) 1010000059UL  
*correlation part of hyb-tau-hcth*  
References:  
*A. D. Boese and N. C. Handy, J. Chem. Phys. 116, 9559 (2002) (10.1063/1.1476309)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_ITYH\\_X](#) 1010000060UL  
*Short-range recipe for exchange GGA functionals*  
References:  
*H. Iikura, T. Tsuneda, T. Yanai, and K. Hirao, J. Chem. Phys. 115, 3540 (2001) (10.1063/1.1383587)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_KGG99\\_X](#) 1010000061UL  
*Gilbert and Gill 1999 (mixed)*  
References:  
*A. T. Gilbert and P. M. Gill, Chem. Phys. Lett. 312, 511 (1999) (10.1016/S0009-2614(99)00836-2)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_KT1\\_X](#) 1010000062UL  
*Exchange part of Keal and Tozer version 1*  
References:  
*T. W. Keal and D. J. Tozer, J. Chem. Phys. 119, 3015 (2003) (10.1063/1.1590634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_KT1\\_XC](#) 1010000063UL  
*Keal and Tozer, version 1*  
References:  
*T. W. Keal and D. J. Tozer, J. Chem. Phys. 119, 3015 (2003) (10.1063/1.1590634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_KT2\\_XC](#) 1010000064UL  
*Keal and Tozer, version 2*  
References:  
*T. W. Keal and D. J. Tozer, J. Chem. Phys. 119, 3015 (2003) (10.1063/1.1590634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LAG\\_X](#) 1010000065UL  
*Local Airy Gas*  
References:  
*L. Vitos, B. Johansson, J. Koll'ar, and H. L. Skriver, Phys. Rev. B 62, 10046 (2000) (10.1103/PhysRevB.62.10046)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LAMBDA\\_CH\\_N\\_X](#) 1010000066UL  
*lambda\_CH(N) version of PBE*  
References:  
*M. M. Odashima, K. Capelle, and S. B. Trickey, J. Chem. Theory Comput. 5, 798 (2009) (10.1021/ct8005634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LAMBDA\\_LO\\_N\\_X](#) 1010000067UL  
*lambda\_LO(N) version of PBE*  
References:  
*M. M. Odashima, K. Capelle, and S. B. Trickey, J. Chem. Theory Comput. 5, 798 (2009) (10.1021/ct8005634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LAMBDA\\_OC2\\_N\\_X](#) 1010000068UL  
*lambda\_OC2(N) version of PBE*  
References:  
*M. M. Odashima, K. Capelle, and S. B. Trickey, J. Chem. Theory Comput. 5, 798 (2009) (10.1021/ct8005634)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LBM\\_X](#) 1010000069UL  
*van Leeuwen & Baerends modified*  
References:  
*P. R. T. Schipper, O. V. Gritsenko, S. J. A. van Gisbergen, and E. J. Baerends, J. Chem. Phys. 112, 1344 (2000) (10.1063/1.480688)*

- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LB\\_X](#) 101000070UL  
*van Leeuwen & Baerends*  
References:  
*R. van Leeuwen and E. J. Baerends, Phys. Rev. A 49, 2421 (1994) (10.1103/PhysRevA.49.2421)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LG93\\_X](#) 101000071UL  
*Lacks & Gordon 93*  
References:  
*D. J. Lacks and R. G. Gordon, Phys. Rev. A 47, 4681 (1993) (10.1103/PhysRevA.47.4681)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LM\\_C](#) 101000072UL  
*Langreth & Mehl*  
References:  
*D. C. Langreth and M. J. Mehl, Phys. Rev. Lett. 47, 446 (1981) (10.1103/PhysRevLett.47.446)*  
*C. D. Hu and D. C. Langreth, Phys. Scr. 32, 391 (1985) (10.1088/0031-8949/32/4/024)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LV\\_RPW86\\_X](#) 101000073UL  
*Berland and Hyldgaard*  
References:  
*K. Berland and P. Hyldgaard, Phys. Rev. B 89, 035412 (2014) (10.1103/PhysRevB.89.035412)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_LYP\\_C](#) 101000074UL  
*Lee, Yang & Parr*  
References:  
*C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B 37, 785 (1988) (10.1103/PhysRevB.37.785)*  
*B. Miehlich, A. Savin, H. Stoll, and H. Preuss, Chem. Phys. Lett. 157, 200 (1989) (10.1016/0009-2614(89)87234-3)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_MB88\\_X](#) 101000075UL  
*Modified Becke 88 for proton transfer*  
References:  
*V. Tognetti and C. Adamo, J. Phys. Chem. A 113, 14415 (2009) (10.1021/jp903672e)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_MOHLYP2\\_XC](#) 101000076UL  
*Functional for barrier heights*  
References:  
*J. Zheng, Y. Zhao, and D. G. Truhlar, J. Chem. Theory Comput. 5, 808 (2009) (10.1021/ct800568m)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_MOHLYP\\_XC](#) 101000077UL  
*Functional for organometallic chemistry*  
References:  
*N. E. Schultz, Y. Zhao, and D. G. Truhlar, J. Phys. Chem. A 109, 11127 (2005) (10.1021/jp0539223)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_MPBE\\_X](#) 101000078UL  
*Adamo & Barone modification to PBE*  
References:  
*C. Adamo and V. Barone, J. Chem. Phys. 116, 5933 (2002) (10.1063/1.1458927)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_MPW91\\_X](#) 101000079UL  
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*Takkar and McCarthy reparametrization*  
References:  
*A. J. Thakkar and S. P. McCarthy, J. Chem. Phys. 131, 134109 (2009) (10.1063/1.3243845)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_TM\\_PBE\\_C](#) 1010000154UL  
*Thakkar and McCarthy reparametrization*  
References:  
*A. J. Thakkar and S. P. McCarthy, J. Chem. Phys. 131, 134109 (2009) (10.1063/1.3243845)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_VMT84\\_GE\\_X](#) 1010000155UL  
*VMT{8,4} with constraint satisfaction with mu = mu\_GE*  
References:  
*A. Vela, J. C. Pacheco-Kato, J. L. G'azquez, J. M. del Campo, and S. B. Trickey, J. Chem. Phys. 136, 144115 (2012) (10.1063/1.3701132)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_VMT84\\_PBE\\_X](#) 1010000156UL  
*VMT{8,4} with constraint satisfaction with mu = mu\_PBE*  
References:  
*A. Vela, J. C. Pacheco-Kato, J. L. G'azquez, J. M. del Campo, and S. B. Trickey, J. Chem. Phys. 136, 144115 (2012) (10.1063/1.3701132)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_VMT\\_GE\\_X](#) 1010000157UL  
*Vela, Medel, and Trickey with mu = mu\_GE*  
References:  
*A. Vela, V. Medel, and S. B. Trickey, J. Chem. Phys. 130, 244103 (2009) (10.1063/1.3152713)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_VMT\\_PBE\\_X](#) 1010000158UL  
*Vela, Medel, and Trickey with mu = mu\_PBE*  
References:  
*A. Vela, V. Medel, and S. B. Trickey, J. Chem. Phys. 130, 244103 (2009) (10.1063/1.3152713)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_VV10\\_XC](#) 1010000159UL  
*Vydrov and Van Voorhis*  
References:  
*O. A. Vydrov and T. Van Voorhis, J. Chem. Phys. 133, 244103 (2010) (10.1063/1.3521275)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_W94\\_C](#) 1010000160UL  
*Wilson 94 (Eq. 25)*  
References:  
*L. C. Wilson, Chemical Physics 181, 337 (1994) (10.1016/0301-0104(93)E0444-Z)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_WC\\_X](#) 1010000161UL  
*Wu & Cohen*  
References:  
*Z. Wu and R. E. Cohen, Phys. Rev. B 73, 235116 (2006) (10.1103/PhysRevB.73.235116)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_WI0\\_C](#) 1010000162UL  
*Wilson & Ivanov initial version*  
References:  
*L. C. Wilson and S. Ivanov, Int. J. Quantum Chem. 69, 523 (1998) (10.1002/(SICI)1097-461X(1998)69:4<523::AID-QUA9>3.0.CO;2-X)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_WI\\_C](#) 1010000163UL  
*Wilson & Ivanov*  
References:  
*L. C. Wilson and S. Ivanov, Int. J. Quantum Chem. 69, 523 (1998) (10.1002/(SICI)1097-461X(1998)69:4<523::AID-QUA9>3.0.CO;2-X)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_WL\\_C](#) 1010000164UL  
*Wilson & Levy*  
References:  
*L. C. Wilson and M. Levy, Phys. Rev. B 41, 12930 (1990) (10.1103/PhysRevB.41.12930)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_WPBEH\\_X](#) 1010000165UL  
*short-range part of the PBE (default w=0 gives PBEh)*  
References:  
*J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003) (10.1063/1.1564060)*  
*J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 124, 219906 (2006) (10.1063/1.2204597)*  
*M. Ernzerhof and J. P. Perdew, J. Chem. Phys. 109, 3313 (1998) (10.1063/1.476928)*  
*J. Heyd and G. E. Scuseria, J. Chem. Phys. 120, 7274 (2004) (10.1063/1.1668634)*

- T. M. Henderson, A. F. Izmaylov, G. Scalmani, and G. E. Scuseria, J. Chem. Phys. 131, 044108 (2009) (10.1063/1.3185673)*
- #define [BRIAN\\_FUNCTIONAL\\_GGA\\_XLYP\\_XC](#) 1010000166UL  
XLYP  
References:  
*X. Xu and W. A. Goddard, Proc. Natl. Acad. Sci. U. S. A. 101, 2673 (2004) (10.1073/pnas.0308730100)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_XPBE\\_C](#) 1010000167UL  
Extended PBE by Xu & Goddard III  
References:  
*X. Xu and W. A. Goddard, J. Chem. Phys. 121, 4068 (2004) (10.1063/1.1771632)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_XPBE\\_X](#) 1010000168UL  
Extended PBE by Xu & Goddard III  
References:  
*X. Xu and W. A. Goddard, J. Chem. Phys. 121, 4068 (2004) (10.1063/1.1771632)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_ZPBEINT\\_C](#) 1010000169UL  
spin-dependent gradient correction to PBEint  
References:  
*L. A. Constantin, E. Fabiano, and F. Della Sala, Phys. Rev. B 84, 233103 (2011) (10.1103/PhysRevB.84.233103)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_ZPBESOL\\_C](#) 1010000170UL  
spin-dependent gradient correction to PBEsol  
References:  
*L. A. Constantin, E. Fabiano, and F. Della Sala, Phys. Rev. B 84, 233103 (2011) (10.1103/PhysRevB.84.233103)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_ZVPBEINT\\_C](#) 1010000171UL  
another spin-dependent correction to PBEint  
References:  
*L. A. Constantin, E. Fabiano, and F. D. Sala, J. Chem. Phys. 137, 194105 (2012) (10.1063/1.4766324)*
  - #define [BRIAN\\_FUNCTIONAL\\_GGA\\_ZVPBESOL\\_C](#) 1010000172UL  
another spin-dependent correction to PBEsol  
References:  
*L. A. Constantin, E. Fabiano, and F. D. Sala, J. Chem. Phys. 137, 194105 (2012) (10.1063/1.4766324)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B1LYP\\_XC](#) 1010000173UL  
B1LYP  
Functional components: 0.25\*HF\_Exchange  
References:  
*C. Adamo and V. Barone, Chem. Phys. Lett. 274, 242 (1997) (10.1016/S0009-2614(97)00651-9)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B1PW91\\_XC](#) 1010000174UL  
B1PW91  
Functional components: 0.25\*HF\_Exchange  
References:  
*C. Adamo and V. Barone, Chem. Phys. Lett. 274, 242 (1997) (10.1016/S0009-2614(97)00651-9)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B1WC\\_XC](#) 1010000175UL  
B1WC  
Functional components: 0.16\*HF\_Exchange  
References:  
*D. I. Bilc, R. Orlando, R. Shaltaf, G.-M. Rignanese, J. Íñiguez, and P. Ghosez, Phys. Rev. B 77, 165107 (2008) (10.1103/PhysRevB.77.165107)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3LYP5\\_XC](#) 1010000176UL  
B3LYP with VWN functional 5 instead of RPA  
Functional components: 0.2\*HF\_Exchange  
References:  
*P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, J. Phys. Chem. 98, 11623 (1994) (10.1021/j100096a001)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3LYPS\\_XC](#) 1010000177UL  
B3LYP\*  
Functional components: 0.15\*HF\_Exchange  
References:  
*M. Reiher, O. Salomon, and B. A. Hess, Theor. Chem. Acc. 107, 48 (2001) (10.1007/s00214-001-0300-3)*
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3LYP\\_LXC\\_XC](#) 1010000178UL  
B3LYP  
Functional components: 0.2\*HF\_Exchange  
References:  
*P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, J. Phys. Chem. 98, 11623 (1994) (10.1021/j100096a001)*

- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3LYP\\_XC](#) 1010000179UL  
*B3LYP*  
*Functional components: 0.2\*HF\_Exchange + 0.08\*LDA\_SLATER\_X + 0.19\*LDA\_VWN1RPA\_C + 0.72\*GGA\*\_B88\_X + 0.81\*GGA\_LYP\_C*  
*References:*  
*P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, J. Phys. Chem. 98, 11623 (1994) (10.1021/j100096a001)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3P86\\_XC](#) 1010000180UL  
*B3P86*  
*Functional components: 0.2\*HF\_Exchange*  
*References:*  
*Defined through Gaussian implementation.*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B3PW91\\_XC](#) 1010000181UL  
*The original (ACM, B3PW91) hybrid of Becke*  
*Functional components: 0.2\*HF\_Exchange*  
*References:*  
*A. D. Becke, J. Chem. Phys. 98, 5648 (1993) (10.1063/1.464913)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B5050LYP\\_XC](#) 1010000182UL  
*B5050LYP*  
*Functional components: 0.5\*HF\_Exchange*  
*References:*  
*Y. Shao, M. Head-Gordon, and A. I. Krylov, J. Chem. Phys. 118, 4807 (2003) (10.1063/1.1545679)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_1P\\_XC](#) 1010000183UL  
*version of B97 by Cohen and Handy*  
*Functional components: 0.15\*HF\_Exchange*  
*References:*  
*A. J. Cohen and N. C. Handy, Chem. Phys. Lett. 316, 160 (2000) (10.1016/S0009-2614(99)01273-7)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_1\\_XC](#) 1010000184UL  
*Becke 97-1*  
*Functional components: 0.21\*HF\_Exchange*  
*References:*  
*F. A. Hamprecht, A. J. Cohen, D. J. Tozer, and N. C. Handy, J. Chem. Phys. 109, 6264 (1998) (10.1063/1.477267)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_2\\_XC](#) 1010000185UL  
*Becke 97-2*  
*Functional components: 0.21\*HF\_Exchange*  
*References:*  
*P. J. Wilson, T. J. Bradley, and D. J. Tozer, J. Chem. Phys. 115, 9233 (2001) (10.1063/1.1412605)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_3\\_XC](#) 1010000186UL  
*Becke 97-3*  
*Functional components: 0.269288\*HF\_Exchange*  
*References:*  
*T. W. Keal and D. J. Tozer, J. Chem. Phys. 123, 121103 (2005) (10.1063/1.2061227)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_K\\_XC](#) 1010000187UL  
*Boese-Martin for Kinetics*  
*Functional components: 0.42\*HF\_Exchange*  
*References:*  
*A. D. Boese and J. M. L. Martin, J. Chem. Phys. 121, 3405 (2004) (10.1063/1.1774975)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_B97\\_XC](#) 1010000188UL  
*Becke 97*  
*Functional components: 0.1943\*HF\_Exchange*  
*References:*  
*A. D. Becke, J. Chem. Phys. 107, 8554 (1997) (10.1063/1.475007)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_BHANDHLYP\\_XC](#) 1010000189UL  
*BHandHLYP*  
*Functional components: 0.5\*HF\_Exchange*  
*References:*  
*A. D. Becke, J. Chem. Phys. 98, 1372 (1993) (10.1063/1.464304)*  
*Defined through Gaussian implementation.*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_BHANDH\\_XC](#) 1010000190UL  
*BHandH*  
*Functional components: 0.5\*HF\_Exchange*  
*References:*

- A. D. Becke, *J. Chem. Phys.* 98, 1372 (1993) (10.1063/1.464304)  
Defined through Gaussian implementation.
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_CAMY\\_B3LYP\\_XC](#) 1010000191UL  
CAMY version of B3LYP  
Functional components:  $0.19*HF\_Exchange\_ShortRange + 0.65*HF\_Exchange\_LongRange$   
References:  
M. Seth and T. Ziegler, *J. Chem. Theory Comput.* 8, 901 (2012) (10.1021/ct300006h)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_CAMY\\_BLYP\\_XC](#) 1010000192UL  
CAMY version of BLYP  
Functional components:  $0.2*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
References:  
Y. Akinaga and S. Ten-no, *Chem. Phys. Lett.* 462, 348 (2008) (10.1016/j.cplett.2008.07.103)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_CAM\\_B3LYP\\_XC](#) 1010000193UL  
CAM version of B3LYP  
Functional components:  $0.19*HF\_Exchange\_ShortRange + 0.65*HF\_Exchange\_LongRange$   
References:  
T. Yanai, D. P. Tew, and N. C. Handy, *Chem. Phys. Lett.* 393, 51 (2004) (10.1016/j.cplett.2004.06.011)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_CAM\\_QTP\\_01\\_XC](#) 1010000194UL  
CAM-B3LYP retuned using ionization potentials of water  
Functional components:  $0.23*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
References:  
Y. Jin and R. J. Bartlett, *J. Chem. Phys.* 145, 034107 (2016), <http://dx.doi.org/10.1063/1.4955497>  
(10.1063/1.4955497)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_CAP0\\_XC](#) 1010000195UL  
Correct Asymptotic Potential hybrid  
Functional components:  $0.25*HF\_Exchange$   
References:  
J. Carmona-Esp'indola, J. L. G'azquez, A. Vela, and S. B. Trickey, *Theor. Chem. Acc.* 135, 120 (2016) (10.1007/s00214-016-1864-2)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_EDF2\\_XC](#) 1010000196UL  
EDF2  
Functional components:  $0.1695*HF\_Exchange$   
References:  
C. Y. Lin, M. W. George, and P. M. W. Gill, *Australian Journal of Chemistry* 57, 365 (2004) (10.1071/CH03263)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HJS\\_B88\\_XC](#) 1010000197UL  
HJS hybrid screened exchange B88 version  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HJS\\_B97X\\_XC](#) 1010000198UL  
HJS hybrid screened exchange B97x version  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HJS\\_PBE\\_SOL\\_XC](#) 1010000199UL  
HJS hybrid screened exchange PBE\_SOL version  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HJS\\_PBE\\_XC](#) 1010000200UL  
HJS hybrid screened exchange PBE version  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
T. M. Henderson, B. G. Janesko, and G. E. Scuseria, *J. Chem. Phys.* 128, 194105 (2008) (10.1063/1.2921797)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HSE03\\_XC](#) 1010000201UL  
HSE03  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* 118, 8207 (2003) (10.1063/1.1564060)  
J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* 124, 219906 (2006) (10.1063/1.2204597)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_HSE06\\_XC](#) 1010000202UL

- HSE06*  
 Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
 References:  
 J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* 118, 8207 (2003) (10.1063/1.1564060)  
 J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* 124, 219906 (2006) (10.1063/1.2204597)  
 A. V. Kruckau, O. A. Vydrov, A. F. Izmaylov, and G. E. Scuseria, *J. Chem. Phys.* 125, 224106 (2006) (10.1063/1.2404663)
- #define BRIAN\_FUNCTIONAL\_HGGA\_HSE12S\_XC 1010000203UL  
*HSE12 (short-range version)*  
 Functional components:  $0.425*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
 References:  
 J. E. Moussa, P. A. Schultz, and J. R. Chelikowsky, *J. Chem. Phys.* 136, 204117 (2012) (10.1063/1.4722993)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_HSE12\_XC 1010000204UL  
*HSE12*  
 Functional components:  $0.313*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
 References:  
 J. E. Moussa, P. A. Schultz, and J. R. Chelikowsky, *J. Chem. Phys.* 136, 204117 (2012) (10.1063/1.4722993)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_HSE\_SOL\_XC 1010000205UL  
*HSEsol*  
 Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
 References:  
 L. Schimka, J. Harl, and G. Kresse, *J. Chem. Phys.* 134, 024116 (2011) (10.1063/1.3524336)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_KMLYP\_XC 1010000206UL  
*Kang-Musgrave hybrid*  
 Functional components:  $0.557*HF\_Exchange$   
 References:  
 J. K. Kang and C. B. Musgrave, *J. Chem. Phys.* 115, 11040 (2001), <http://dx.doi.org/10.1063/1.1415079> (10.1063/1.1415079)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LCY\_BLYP\_XC 1010000207UL  
*LCY version of BLYP*  
 Functional components:  $0*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 Y. Akinaga and S. Ten-no, *Chem. Phys. Lett.* 462, 348 (2008) (10.1016/j.cplett.2008.07.103)  
 M. Seth, T. Ziegler, M. Steinmetz, and S. Grimme, *J. Chem. Theory Comput.* 9, 2286 (2013) (10.1021/ct301112m)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LCY\_PBE\_XC 1010000208UL  
*LCY version of PBE*  
 Functional components:  $0*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 M. Seth and T. Ziegler, *J. Chem. Theory Comput.* 8, 901 (2012) (10.1021/ct300006h)  
 M. Seth, T. Ziegler, M. Steinmetz, and S. Grimme, *J. Chem. Theory Comput.* 9, 2286 (2013) (10.1021/ct301112m)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LC\_VV10\_XC 1010000209UL  
*Vydrov and Van Voorhis*  
 Functional components:  $0*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 O. A. Vydrov and T. Van Voorhis, *J. Chem. Phys.* 133, 244103 (2010) (10.1063/1.3521275)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LC\_WPBE\_XC 1010000210UL  
*Long-range corrected PBE (LC-wPBE) by Vydrov and Scuseria*  
 Functional components:  $0*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 O. A. Vydrov and G. E. Scuseria, *J. Chem. Phys.* 125, 234109 (2006), 10.1063/1.2409292 (10.1063/1.2409292)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LRC\_WPBEH\_XC 1010000211UL  
*Long-range corrected short-range hybrid PBE (LRC-wPBEh) by Rohrdanz, Martins and Herbert*  
 Functional components:  $0.2*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 M. A. Rohrdanz, K. M. Martins, and J. M. Herbert, *J. Chem. Phys.* 130, 054112 (2009) (10.1063/1.3073302)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_LRC\_WPBE\_XC 1010000212UL  
*Long-range corrected PBE (LRC-wPBE) by Rohrdanz, Martins and Herbert*  
 Functional components:  $0*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
 References:  
 M. A. Rohrdanz, K. M. Martins, and J. M. Herbert, *J. Chem. Phys.* 130, 054112 (2009) (10.1063/1.3073302)
  - #define BRIAN\_FUNCTIONAL\_HGGA\_MB3LYP\_RC04\_XC 1010000213UL



- B3LYP with RC04 LDA*  
 Functional components: 0.2\*HF\_Exchange  
 References:  
 V. Tognetti, P. Cortona, and C. Adamo, *Chem. Phys. Lett.* 439, 381 (2007) (10.1016/j.cplett.2007.03.081)
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW1K\\_XC](#) 1010000214UL  
*mPW1K*  
 Functional components: 0.428\*HF\_Exchange  
 References:  
 B. J. Lynch, P. L. Fast, M. Harris, and D. G. Truhlar, *J. Phys. Chem. A* 104, 4811 (2000) (10.1021/jp000497z)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW1LYP\\_XC](#) 1010000215UL  
*mPW1LYP*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 C. Adamo and V. Barone, *J. Chem. Phys.* 108, 664 (1998) (10.1063/1.475428)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW1PBE\\_XC](#) 1010000216UL  
*mPW1PBE*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 C. Adamo and V. Barone, *J. Chem. Phys.* 108, 664 (1998) (10.1063/1.475428)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW1PW\\_XC](#) 1010000217UL  
*mPW1PW*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 C. Adamo and V. Barone, *J. Chem. Phys.* 108, 664 (1998) (10.1063/1.475428)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW3LYP\\_XC](#) 1010000218UL  
*MPW3LYP*  
 Functional components: 0.218\*HF\_Exchange  
 References:  
 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 108, 6908 (2004) (10.1021/jp048147q)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPW3PW\\_XC](#) 1010000219UL  
*MPW3PW of Adamo & Barone*  
 Functional components: 0.2\*HF\_Exchange  
 References:  
 C. Adamo and V. Barone, *J. Chem. Phys.* 108, 664 (1998) (10.1063/1.475428)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_MPWLYP1M\\_XC](#) 1010000220UL  
*MPW with 1 par. for metals/LYP*  
 Functional components: 0.05\*HF\_Exchange  
 References:  
 N. E. Schultz, Y. Zhao, and D. G. Truhlar, *J. Phys. Chem. A* 109, 11127 (2005) (10.1021/jp0539223)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_N12\\_SX\\_X](#) 1010000221UL  
*Minnesota N12-SX exchange functional*  
 Functional components: 0.25\*HF\_Exchange\_ShortRange + 0\*HF\_Exchange\_LongRange  
 References:  
 R. Peverati and D. G. Truhlar, *Phys. Chem. Chem. Phys.* 14, 16187 (2012) (10.1039/C2CP42576A)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_O3LYP\\_XC](#) 1010000222UL  
*O3LYP*  
 Functional components: 0.1161\*HF\_Exchange  
 References:  
 A. J. Cohen and N. C. Handy, *Mol. Phys.* 99, 607 (2001) (10.1080/00268970010023435)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_PBE0\\_13\\_XC](#) 1010000223UL  
*PBE0-1/3*  
 Functional components: 0.333333\*HF\_Exchange  
 References:  
 P. Cortona, *J. Chem. Phys.* 136, 086101 (2012) (10.1063/1.3690462)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_PBE50\\_XC](#) 1010000224UL  
*PBE50*  
 Functional components: 0.5\*HF\_Exchange  
 References:  
 Y. A. Bernard, Y. Shao, and A. I. Krylov, *J. Chem. Phys.* 136, 204103 (2012) (10.1063/1.4714499)
  - #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_PBEB0\\_XC](#) 1010000225UL  
*PBEbeta0*  
 Functional components: 0.25\*HF\_Exchange

- References:  
*J. M. del Campo, J. L. G\’azquez, S. B. Trickey, and A. Vela, J. Chem. Phys. 136, 104108 (2012) (10.1063/1.3691197)*
- #define BRIAN\_FUNCTIONAL\_HGGA\_PBEH\_XC 1010000226UL  
 PBEH (PBE0)  
 Functional components: 0.25\*HF\_Exchange  
 References:  
*C. Adamo and V. Barone, J. Chem. Phys. 110, 6158 (1999) (10.1063/1.478522)*  
*M. Ernzerhof and G. E. Scuseria, J. Chem. Phys. 110, 5029 (1999) (10.1063/1.478401)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_PBE\_MOLO\_XC 1010000227UL  
 PBE<sub>mol0</sub>  
 Functional components: 0.25\*HF\_Exchange  
 References:  
*J. M. del Campo, J. L. G\’azquez, S. B. Trickey, and A. Vela, J. Chem. Phys. 136, 104108 (2012) (10.1063/1.3691197)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_PBE\_MOLB0\_XC 1010000228UL  
 PBE<sub>molbeta0</sub>  
 Functional components: 0.25\*HF\_Exchange  
 References:  
*J. M. del Campo, J. L. G\’azquez, S. B. Trickey, and A. Vela, J. Chem. Phys. 136, 104108 (2012) (10.1063/1.3691197)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_PBE\_SOLO\_XC 1010000229UL  
 PBE<sub>sol0</sub>  
 Functional components: 0.25\*HF\_Exchange  
 References:  
*J. M. del Campo, J. L. G\’azquez, S. B. Trickey, and A. Vela, J. Chem. Phys. 136, 104108 (2012) (10.1063/1.3691197)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_REVB3LYP\_XC 1010000230UL  
 Revised B3LYP  
 Functional components: 0.2\*HF\_Exchange  
 References:  
*L. Lu, H. Hu, H. Hou, and B. Wang, Comput. Theor. Chem. 1015, 64 (2013) (10.1016/j.comptc.2013.04.009)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_1A\_XC 1010000231UL  
 SB98 (1a)  
 Functional components: 0.229015\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_1B\_XC 1010000232UL  
 SB98 (1b)  
 Functional components: 0.199352\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_1C\_XC 1010000233UL  
 SB98 (1c)  
 Functional components: 0.192416\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_2A\_XC 1010000234UL  
 SB98 (2a)  
 Functional components: 0.232055\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_2B\_XC 1010000235UL  
 SB98 (2b)  
 Functional components: 0.237978\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*
  - #define BRIAN\_FUNCTIONAL\_HGGA\_SB98\_2C\_XC 1010000236UL  
 SB98 (2c)  
 Functional components: 0.219847\*HF\_Exchange  
 References:  
*H. L. Schmider and A. D. Becke, J. Chem. Phys. 108, 9624 (1998) (10.1063/1.476438)*

- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_SOGGA11\\_X\\_X](#) 1010000237UL  
*Hybrid based on SOGGA11 form*  
*Functional components: 0.4015\*HF\_Exchange*  
*References:*  
*R. Peverati and D. G. Truhlar, J. Chem. Phys. 135, 191102 (2011) (10.1063/1.3663871)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_TUNED\\_CAM\\_B3LYP\\_XC](#) 1010000238UL  
*CAM version of B3LYP, tuned for excitations and properties*  
*Functional components: 0.0799\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange*  
*References:*  
*K. Okuno, Y. Shigeta, R. Kishi, H. Miyasaka, and M. Nakano, J. Photochem. Photobiol., A 235, 29 (2012) (10.1016/j.jphotochem.2012.03.003)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_WB97X\\_D\\_XC](#) 1010000239UL  
*wB97D range-separated functional*  
*Functional components: 0.222036\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange*  
*References:*  
*J.-D. Chai and M. Head-Gordon, Phys. Chem. Chem. Phys. 10, 6615 (2008) (10.1039/B810189B)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_WB97X\\_V\\_XC](#) 1010000240UL  
*wB97X-V range-separated functional*  
*Functional components: 0.167\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange*  
*References:*  
*N. Mardirossian and M. Head-Gordon, Phys. Chem. Chem. Phys. 16, 9904 (2014) (10.1039/C3CP54374A)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_WB97X\\_XC](#) 1010000241UL  
*wB97X range-separated functional*  
*Functional components: 0.157706\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange*  
*References:*  
*J.-D. Chai and M. Head-Gordon, J. Chem. Phys. 128, 084106 (2008) (10.1063/1.2834918)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_WB97\\_XC](#) 1010000242UL  
*wB97 range-separated functional*  
*Functional components: 0\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange*  
*References:*  
*J.-D. Chai and M. Head-Gordon, J. Chem. Phys. 128, 084106 (2008) (10.1063/1.2834918)*
- #define [BRIAN\\_FUNCTIONAL\\_HGGA\\_X3LYP\\_XC](#) 1010000243UL  
*X3LYP*  
*Functional components: 0.218\*HF\_Exchange*  
*References:*  
*X. Xu and W. A. Goddard, Proc. Natl. Acad. Sci. U. S. A. 101, 2673 (2004) (10.1073/pnas.0308730100)*
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_B86B95\\_XC](#) 1010000244UL  
*Mixture of B86 with BC95*  
*Functional components: 0.28\*HF\_Exchange*  
*References:*  
*A. D. Becke, J. Chem. Phys. 104, 1040 (1996) (10.1063/1.470829)*
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_B88B95\\_XC](#) 1010000245UL  
*Mixture of B88 with BC95 (B1B95)*  
*Functional components: 0.28\*HF\_Exchange*  
*References:*  
*A. D. Becke, J. Chem. Phys. 104, 1040 (1996) (10.1063/1.470829)*
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_BB1K\\_XC](#) 1010000246UL  
*Mixture of B88 with BC95 from Zhao and Truhlar*  
*Functional components: 0.42\*HF\_Exchange*  
*References:*  
*Y. Zhao, B. J. Lynch, and D. G. Truhlar, J. Phys. Chem. A 108, 2715 (2004) (10.1021/jp049908s)*
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_BMK\\_X](#) 1010000247UL  
*Boese-Martin for kinetics*  
*Functional components: 0.42\*HF\_Exchange*  
*References:*  
*A. D. Boese and J. M. L. Martin, J. Chem. Phys. 121, 3405 (2004) (10.1063/1.1774975)*
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_DLDF\\_X](#) 1010000248UL  
*Dispersionless Density Functional*  
*Functional components: 0.614413\*HF\_Exchange*  
*References:*  
*K. Pernal, R. Podeszwa, K. Patkowski, and K. Szalewicz, Phys. Rev. Lett. 103, 263201 (2009) (10.1103/PhysRevLett.103.263201)*

- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M05\\_2X\\_X](#) 1010000249UL  
Minnesota M05-2X hybrid exchange functional  
Functional components:  $0.56*HF\_Exchange$   
References:  
Y. Zhao, N. E. Schultz, and D. G. Truhlar, *J. Chem. Theory Comput.* 2, 364 (2006) (10.1021/ct0502763)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M05\\_X](#) 1010000250UL  
Minnesota M05 hybrid exchange functional  
Functional components:  $0.28*HF\_Exchange$   
References:  
Y. Zhao, N. E. Schultz, and D. G. Truhlar, *J. Chem. Phys.* 123, 161103 (2005) (10.1063/1.2126975)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M06\\_2X\\_X](#) 1010000251UL  
Minnesota M06-2X hybrid exchange functional  
Functional components:  $0.54*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* 120, 215 (2008) (10.1007/s00214-007-0310-x)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M06\\_HF\\_X](#) 1010000252UL  
Minnesota M06-HF hybrid exchange functional  
Functional components:  $HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 110, 13126 (2006) (10.1021/jp066479k)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M06\\_X](#) 1010000253UL  
Minnesota M06 hybrid exchange functional  
Functional components:  $0.27*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* 120, 215 (2008) (10.1007/s00214-007-0310-x)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M08\\_HX\\_X](#) 1010000254UL  
Minnesota M08-HX hybrid exchange functional  
Functional components:  $0.5223*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.* 4, 1849 (2008) (10.1021/ct800246v)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M08\\_SO\\_X](#) 1010000255UL  
Minnesota M08-SO hybrid exchange functional  
Functional components:  $0.5679*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.* 4, 1849 (2008) (10.1021/ct800246v)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_M11\\_X](#) 1010000256UL  
Minnesota M11 hybrid exchange functional  
Functional components:  $0.428*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange$   
References:  
R. Peverati and D. G. Truhlar, *J. Phys. Chem. Lett.* 2, 2810 (2011) (10.1021/jz201170d)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MN12\\_SX\\_X](#) 1010000257UL  
Minnesota MN12-SX hybrid exchange functional  
Functional components:  $0.25*HF\_Exchange\_ShortRange + 0*HF\_Exchange\_LongRange$   
References:  
R. Peverati and D. G. Truhlar, *Phys. Chem. Chem. Phys.* 14, 16187 (2012) (10.1039/C2CP42576A)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MN15\\_X](#) 1010000258UL  
Minnesota MN15 hybrid exchange functional  
Functional components:  $0.44*HF\_Exchange$   
References:  
H. S. Yu, X. He, S. L. Li, and D. G. Truhlar, *Chem. Sci.* 7, 5032 (2016) (10.1039/C6SC00705H)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MPW1B95\\_XC](#) 1010000259UL  
Mixture of mPW91 with BC95 from Zhao and Truhlar  
Functional components:  $0.31*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 108, 6908 (2004) (10.1021/jp048147q)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MPWB1K\\_XC](#) 1010000260UL  
Mixture of mPW91 with BC95 for kinetics  
Functional components:  $0.44*HF\_Exchange$   
References:  
Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 108, 6908 (2004) (10.1021/jp048147q)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MS2H\\_X](#) 1010000261UL

- MS2 hybrid exchange of Sun, et al*  
 Functional components: 0.09\*HF\_Exchange  
 References:  
 J. Sun, R. Haunschild, B. Xiao, I. W. Bulik, G. E. Scuseria, and J. P. Perdew, *J. Chem. Phys.* 138, 044113 (2013) (10.1063/1.4789414)
- #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_MVSH\\_X](#) 1010000262UL  
*MVSh hybrid exchange functional*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 J. Sun, J. P. Perdew, and A. Ruzsinszky, *Proc. Natl. Acad. Sci. U. S. A.* 112, 685 (2015) (10.1073/pnas.1423145112)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_PW6B95\\_XC](#) 1010000263UL  
*Mixture of PW91 with BC95 from Zhao and Truhlar*  
 Functional components: 0.28\*HF\_Exchange  
 References:  
 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 109, 5656 (2005) (10.1021/jp050536c)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_PW86B95\\_XC](#) 1010000264UL  
*Mixture of PW86 with BC95*  
 Functional components: 0.29\*HF\_Exchange  
 References:  
 A. D. Becke, *J. Chem. Phys.* 104, 1040 (1996) (10.1063/1.470829)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_PWB6K\\_XC](#) 1010000265UL  
*Mixture of PW91 with BC95 from Zhao and Truhlar for kinetics*  
 Functional components: 0.46\*HF\_Exchange  
 References:  
 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 109, 5656 (2005) (10.1021/jp050536c)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_REVSCAN0\\_X](#) 1010000266UL  
*revised SCAN hybrid exchange (SCAN0)*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 P. D. Mezei, G. I. Csonka, and M. Kállay, *J. Chem. Theory Comput.* 0, null (0) (10.1021/acs.jctc.8b00072)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_REVTPSSH\\_XC](#) 1010000267UL  
*revTPSSH*  
 Functional components: 0.1\*HF\_Exchange  
 References:  
 G. I. Csonka, J. P. Perdew, and A. Ruzsinszky, *J. Chem. Theory Comput.* 6, 3688 (2010) (10.1021/ct100488v)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_SCAN0\\_X](#) 1010000268UL  
*SCAN hybrid exchange (SCAN0)*  
 Functional components: 0.25\*HF\_Exchange  
 References:  
 K. Hui and J.-D. Chai, *J. Chem. Phys.* 144, 044114 (2016), 10.1063/1.4940734 (10.1063/1.4940734)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_TAU\\_HCTH\\_X](#) 1010000269UL  
*Hybrid version of tau-HCTH*  
 Functional components: 0.15\*HF\_Exchange  
 References:  
 A. D. Boese and N. C. Handy, *J. Chem. Phys.* 116, 9559 (2002) (10.1063/1.1476309)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_TPSSH\\_XC](#) 1010000270UL  
*TPSSH*  
 Functional components: 0.1\*HF\_Exchange  
 References:  
 V. N. Staroverov, G. E. Scuseria, J. Tao, and J. P. Perdew, *J. Chem. Phys.* 119, 12129 (2003) (10.1063/1.1626543)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_WB97M\\_V\\_XC](#) 1010000271UL  
*wB97M-V exchange-correlation functional*  
 Functional components: 0.15\*HF\_Exchange\_ShortRange + HF\_Exchange\_LongRange  
 References:  
 N. Mardirossian and M. Head-Gordon, *J. Chem. Phys.* 144, 214110 (2016) (10.1063/1.4952647)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_X1B95\\_XC](#) 1010000272UL  
*Mixture of X with BC95*  
 Functional components: 0.3\*HF\_Exchange  
 References:  
 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 108, 6908 (2004) (10.1021/jp048147q)
  - #define [BRIAN\\_FUNCTIONAL\\_HMGGA\\_XB1K\\_XC](#) 1010000273UL

- Mixture of X with BC95 for kinetics  
 Functional components: 0.43\*HF\_Exchange  
 References:  
 Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A* 108, 6908 (2004) (10.1021/jp048147q)
- #define BRIAN\_FUNCTIONAL\_LDA\_BR78\_C 1010000274UL  
 Brual & Rothstein 78  
 References:  
 G. B. Jr. and S. M. Rothstein, *J. Chem. Phys.* 69, 1177 (1978) (10.1063/1.436705)
  - #define BRIAN\_FUNCTIONAL\_LDA\_CHACHIYO\_C 1010000275UL  
 Chachiyo simple 2 parameter correlation  
 References:  
 T. Chachiyo, *J. Chem. Phys.* 145, 021101 (2016) (10.1063/1.4958669)
  - #define BRIAN\_FUNCTIONAL\_LDA\_ERF\_X 1010000276UL  
 Attenuated exchange LDA (erf)  
 References:  
 J. Toulouse, A. Savin, and H.-J. Flad, *Int. J. Quantum Chem.* 100, 1047 (2004) (10.1002/qua.20259)  
 Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai, and K. Hirao, *J. Chem. Phys.* 120, 8425 (2004) (10.1063/1.1688752)
  - #define BRIAN\_FUNCTIONAL\_LDA\_GDSMFB\_XC 1010000277UL  
 Groth, Dornheim, Sjostrom, Malone, Foulkes, Bonitz  
 References:  
 S. {Groth}, T. {Dornheim}, T. {Sjostrom}, F. D. {Malone}, W. M. C. {Foulkes}, and M. {Bonitz}, *ArXiv e-prints* (2017), arXiv:1703.08074 [physics.plasm-ph].
  - #define BRIAN\_FUNCTIONAL\_LDA\_GK72\_C 1010000278UL  
 Gordon and Kim 1972  
 References:  
 R. G. Gordon and Y. S. Kim, *J. Chem. Phys.* 56, 3122 (1972), <https://doi.org/10.1063/1.1677649> (10.1063/1.1677649)
  - #define BRIAN\_FUNCTIONAL\_LDA\_GL\_C 1010000279UL  
 Gunnarson & Lundqvist  
 References:  
 O. Gunnarsson and B. I. Lundqvist, *Phys. Rev. B* 13, 4274 (1976) (10.1103/PhysRevB.13.4274)
  - #define BRIAN\_FUNCTIONAL\_LDA\_GOMBAS\_C 1010000280UL  
 Gombas  
 References:  
 P. Gombas, *Pseudopotentiale* (Springer-Verlag, Wien, New York, 1967)
  - #define BRIAN\_FUNCTIONAL\_LDA\_HL\_C 1010000281UL  
 Hedin & Lundqvist  
 References:  
 L. Hedin and B. I. Lundqvist, *J. Phys. C: Solid State Phys.* 4, 2064 (1971) (10.1088/0022-3719/4/14/022)
  - #define BRIAN\_FUNCTIONAL\_LDA\_KARASIEV\_C 1010000282UL  
 Karasiev reparameterization of Chachiyo  
 References:  
 V. V. Karasiev, *J. Chem. Phys.* 145, 157101 (2016), <https://doi.org/10.1063/1.4964758> (10.1063/1.4964758)
  - #define BRIAN\_FUNCTIONAL\_LDA\_KSDT\_XC 1010000283UL  
 Karasiev, Sjostrom, Dufty & Trickey  
 References:  
 V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, *Phys. Rev. Lett.* 112, 076403 (2014) (10.1103/PhysRevLett.112.076403)
  - #define BRIAN\_FUNCTIONAL\_LDA\_LP96\_C 1010000284UL  
 Liu-Parr correlation  
 References:  
 S. Liu and R. G. Parr, *Phys. Rev. A* 53, 2211 (1996) (10.1103/PhysRevA.53.2211)  
 S. Liu and R. Parr, *Journal of Molecular Structure:THEOCHEM* 501–502, 29 (2000) (10.1016/S0166-1280(99)00410-8)
  - #define BRIAN\_FUNCTIONAL\_LDA\_LP\_A\_XC 1010000285UL  
 Lee-Parr reparametrization A  
 References:  
 C. Lee and R. G. Parr, *Phys. Rev. A* 42, 193 (1990) (10.1103/PhysRevA.42.193)
  - #define BRIAN\_FUNCTIONAL\_LDA\_LP\_B\_XC 1010000286UL

- Lee-Parr reparametrization B*  
References:  
C. Lee and R. G. Parr, *Phys. Rev. A* 42, 193 (1990) (10.1103/PhysRevA.42.193)
- #define BRIAN\_FUNCTIONAL\_LDA\_MCWEENY\_C 1010000287UL  
*McWeeny 76*  
References:  
R. McWeeny, in *The New World of Quantum Chemistry*, edited by {editor {B. Pullman} and R. Parr} (Reidel, Boston, 1976) pp. 3–31  
G. B. Jr. and S. M. Rothstein, *J. Chem. Phys.* 69, 1177 (1978) (10.1063/1.436705)
  - #define BRIAN\_FUNCTIONAL\_LDA\_ML1\_C 1010000288UL  
*Modified LSD (version 1) of Proynov and Salahub*  
References:  
E. I. Proynov and D. R. Salahub, *Phys. Rev. B* 49, 7874 (1994) (10.1103/PhysRevB.49.7874)
  - #define BRIAN\_FUNCTIONAL\_LDA\_ML2\_C 1010000289UL  
*Modified LSD (version 2) of Proynov and Salahub*  
References:  
E. I. Proynov and D. R. Salahub, *Phys. Rev. B* 49, 7874 (1994) (10.1103/PhysRevB.49.7874)
  - #define BRIAN\_FUNCTIONAL\_LDA\_OB\_PW\_C 1010000290UL  
*Ortiz & Ballone (PW parametrization)*  
References:  
G. Ortiz and P. Ballone, *Phys. Rev. B* 50, 1391 (1994) (10.1103/PhysRevB.50.1391)  
G. Ortiz and P. Ballone, *Phys. Rev. B* 56, 9970 (1997) (10.1103/PhysRevB.56.9970)  
J. P. Perdew and Y. Wang, *Phys. Rev. B* 45, 13244 (1992), added extra digits to some constants as in the PBE routine (<http://dft.rutgers.edu/pubs/PBE.asc>) (10.1103/PhysRevB.45.13244)
  - #define BRIAN\_FUNCTIONAL\_LDA\_OB\_PZ\_C 1010000291UL  
*Ortiz & Ballone (PZ parametrization)*  
References:  
G. Ortiz and P. Ballone, *Phys. Rev. B* 50, 1391 (1994) (10.1103/PhysRevB.50.1391)  
G. Ortiz and P. Ballone, *Phys. Rev. B* 56, 9970 (1997) (10.1103/PhysRevB.56.9970)
  - #define BRIAN\_FUNCTIONAL\_LDA\_OW\_C 1010000292UL  
*Optimized Wigner*  
References:  
P. A. Stewart and P. M. W. Gill, *J. Chem. Soc., Faraday Trans. 91*, 4337 (1995) (10.1039/FT9959104337)
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  - #define BRIAN\_FUNCTIONAL\_LDA\_PW\_MOD\_C 1010000296UL  
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  - #define BRIAN\_FUNCTIONAL\_LDA\_VWN\_C 1010000316UL  
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