

UNPUBLISHED ERRATUM

"Revised M06 Density Functional for Main-Group and Transition-Metal Chemistry," Y. Wang, P. Verma, X. Jin, D. G. Truhlar, and X. He, *Proceedings of the National Academy of Sciences U.S.A.* **115**, 10257-10262 (2018). doi.org/10.1073/pnas.1810421115

UNPUBLISHED ERRATUM FOR THE SI APPENDIX

The second and last columns of Table S20 (on page S-35 to S-37) were too narrow, and as a consequence some of the entries got truncated. The corrections are:

page	row	old text	corrected text.
S-36	TPSSh	global-hybrid	global-hybrid meta-GGA
S-36	BB1K	(105,124,	(105,124,137)
S-37	PW6B95-D3(BJ)	[blank in second column]	global-hybrid meta-GGA + MM <sup>e</sup>
S-37	M11	RS-hybrid	RS-hybrid meta-GGA <sup>d</sup>
S-37	MN12-SX	RS-hybrid	RS-hybrid meta-NGA <sup>d</sup>
S-37	MN15	global-hybrid	global-hybrid meta-NGA

For convenience, a corrected table is included starting on the next page.

**Table S20 corrected.**

**Table S20. Exchange–correlation functionals tested in this study(1-4, 7-10, 62, 71-137)**

Category	Type	Abbrev.	$X^a$	Year	Method	Ref.		
local	LSDA	LSDA	0	1980	GKSVWN5 <sup>b</sup>	(72-75)		
			0	1980	GKSVWN3 <sup>b</sup>	(72-75)		
	GGA – SO <sup>c</sup> orderexchange	GGA	0	2008	SOGGA	(76)		
			0	2008	PBEsol	(77)		
			0	2011	SOGGA11	(78)		
			GGA – other	GGA	0	1986	B86P86	(79, 80)
					0	1987	B86LYP	(79, 81)
					0	1988	BP86	(80, 137)
					0	1988	BLYP	(81, 137)
					0	1989	BR89LYP	(71, 81)
					0	1991	B86PW91	(79, 82)
					0	1991	PW91 <sup>c</sup>	(82)
	0	1991			BPW91	(82, 137)		
	0	1996			PBE	(4)		
	0	1997			mPWPW	(83)		
	0	1997	revPBE	(84)				
	0	1999	RPBE	(85)				
	0	2001	HCTH407	(86)				
	0	2001	OLYP	(81, 87)				
	0	2001	OPBE	(4, 87, 88)				
	0	2005	MPWLYP1W	(89)				
	0	2005	PBE1W	(89)				
	0	2005	PBELYP1W	(89)				
	0	2005	MOHLYP	(62)				
	0	2006	B97-D	(90)				
	0	2009	MOHLYP2	(91)				
	0	2009	OreLYP	(81, 87, 92)				
	meta-GGA	NGA	NGA	0	2012	N12	(93)	
				0	2015	GAM	(9)	
		meta-GGA	mGGA	0	1998	VSXC	(2)	
				0	2002	$\tau$ -HCTH	(94)	
				0	2003	TPSS	(95)	
				0	2005	TPSSLYP1W	(89)	
0				2006	M06-L	(96)		
0				2009	revTPSS	(97)		
0				2011	M11-L	(98)		
0				2013	MGGA_MS0	(99)		
0	2013	MGGA_MS1	(99)					

			0	2013	MGGA_MS2	(99)
	meta-NGA	mNGA	0	2017	revM06-L	(1)
			0	2012	MN12-L	(100)
			0	2015	MN15-L	(8)
nonlocal	global-hybrid GGA	GGAh	100	1987	HFLYP	(81, 101)
			100	1991	HFPW91	(82, 101)
			20	1992	B3PW91	(102, 137)
			20	1994	B3LYP	(81, 103, 137)
			25	1996	PBE0	(104)
			28	1996	B1B95	(105)
			25	1997	mPW1PW	(83)
			25	1997	B1LYP	(106)
			21.98	1998	B98	(107)
			21	1998	B97-1	(108)
			42.80	2000	MPW1K	(109)
			11.61	2001	O3LYP	(88)
			21	2001	B97-2	(110)
			15	2001	B3LYP*	(111)
			21.8	2004	X3LYP	(112)
			21.8	2004	MPW3LYP	(113)
			5	2005	MPWLYP1M	(62)
			26.93	2005	B97-3	(114)
	RS-hybrid GGA <sup>d</sup>	GGA <sub>rsh</sub>	35.42	2011	SOGGA11-X	(115)
			19-65	2004	CAM-B3LYP	(116)
			0-100	2006	LC- $\omega$ PBE	(133-136)
			25-0	2006	HSE06	(117, 118)
			0-60-0	2008	HISS	(119)
			0-100	2008	$\omega$ B97	(120)
			15.77-	2008	$\omega$ B97X	(120)
	RS-hybrid NGA	NGA <sub>rsh</sub>	25-0	2012	N12-SX	(121)
	RS-hybrid GGA + MM <sup>e</sup>	NGA <sub>rsh</sub> -D	22.2-100	2008	$\omega$ B97X-D	(122)
	global-hybrid meta-GGA	mGGAh	10	2002	TPSSh	(123)
			15	2002	$\tau$ -HCTHhyb	(94)
			42	2004	BB1K	(105, 124, 137)
			44	2004	MPWB1K	(113)
			31	2004	MPW1B95	(113)
			42	2004	BMK	(125)
			13	2005	TPSS1KCIS	(126)
			41	2005	MPWKCIS1K	(91)
			15	2005	MPW1KCIS	(91)
			22	2005	PBE1KCIS	(127)
			46	2005	PWB6K	(128)
			28	2005	PW6B95	(128)

		28	2005	M05	(3)
		56	2005	M05-2X	(7)
		100	2006	M06-HF	(129)
		27	2008	M06	(130)
		54	2008	M06-2X	(130)
		52.23	2008	M08-HX	(131)
		56.79	2008	M08-SO	(131)
		9	2013	MGGA_MS2H	(99)
		40.41	2018	revM06	present
global-hybrid meta-GGA+MM <sup>e</sup>	mGGAh-D	28	2005	PW6B95-D3(BJ)	(128)
RS-hybrid meta-GGA <i>d</i>	mGGArsh	42.8-100	2011	M11	(132)
RS-hybrid meta-NGA	mNGArsh	25-0	2012	MN12-SX	(121)
global-hybrid meta-NGA	mNGAh	44	2015	MN15	(10)