Supplemental Material for
Generalized Gradient Approximations with Local Parameters

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I. FUNCTIONAL DERIVATIVE FORM

For convenience, we point out a modest technical distinction about execution of functional derivatives for the forms under study.

The exchange contribution to the total Kohn-Sham energy for the usual generalized gradient approximations (GGAs) can be expressed in general as

$$E_x\left[n\right] = \int n\left(\mathbf{r}\right)\varepsilon_x\left(\mathbf{r}\right)\, F_x\left(s\right) = \int e_x\left(\mathbf{r}\right)d\mathbf{r}, \tag{1}$$

where $F_x\left(s\right)$ is the enhancement factor that describes deviations from local homogeneous electron gas behavior. Typically it is expressed as an analytic function of the dimensionless gradient $s = \left|\nabla n\left(\mathbf{r}\right)\right| / \left[2\left(3\,\pi^2\,n\left(\mathbf{r}\right)\right)^{1/3} n\left(\mathbf{r}\right)\right]$, as well as depending on several fixed parameters. If the density dependence is written solely in terms of $n(\mathbf{r})$ and its spatial derivatives, then $\delta E_x\left[n\right]/\delta n\left(\mathbf{r}\right) = \partial e_x\left(\mathbf{r}\right)/\partial n\left(\mathbf{r}\right)$, and the corresponding exchange potential is

$$\frac{\partial e_x}{\partial n\left(\mathbf{r}\right)} = \frac{4}{3}\,\varepsilon_x\left(\mathbf{r}\right)\left(F_x - s\frac{\partial F_x}{\partial s}\right), \tag{2}$$

with $\varepsilon_x\left(\mathbf{r}\right)$ defined as

$$\varepsilon_x\left(\mathbf{r}\right) = -\frac{3}{4}\left(\frac{3\,n\left(\mathbf{r}\right)}{\pi}\right)^{1/3}. \tag{3}$$

On the other hand, if the density dependence of the enhancement function also is written, for convenience, in terms of the Wigner-Seitz radius,

$$r_s = \left(\frac{3}{4\,\pi\,n\left(\mathbf{r}\right)}\right)^{1/3}, \tag{4}$$

then the expression for the potential becomes

$$\frac{\partial e_x}{\partial n\left(\mathbf{r}\right)} = \frac{4}{3}\,\varepsilon_x\left(\mathbf{r}\right)\left(F_x - s\frac{\partial F_x}{\partial s} - \frac{1}{4}r_s\frac{\partial F_x}{\partial r_s}\right). \tag{5}$$

II. COEFFICIENT RELATIONSHIPS

For the approximations introduced in Section II of the main paper, the sets of $\beta(r_s)$, $C(r_s)$ and $\mu(r_s)$ take the following forms:

$$\beta_{rev}\left(r_s\right) = \beta_{MB}\,\frac{1 + c_1\, r_s}{1 + c_2\, r_s}, \tag{6}$$

$$\beta_{mod/HL}\left(r_s\right) = \beta_{MB}\,\frac{1 + c_1\, r_s\left(c_2 + c_3\, r_s\right)}{1 + c_1\, r_s\left(1 + c_4\, r_s\right)}, \tag{7}$$

$$\beta_{RG}(r_s) = 16\left(\frac{3}{\pi}\right)^{1/3} C_{RG}(r_s), \tag{8}$$

$$\tag{9}$$

$$C_{rev}(r_s) = \frac{1}{16}\left(\frac{3}{\pi}\right)^{-1/3} \beta_{rev}\left(r_s\right), \tag{10}$$

$$C_{mod/HL}(r_s) = \frac{1}{16}\left(\frac{3}{\pi}\right)^{-1/3} \beta_{mod/HL}\left(r_s\right), \tag{11}$$

$$C_{RG}(r_s) = c_1 + \frac{c_2 + c_3\, r_s + c_4\, r_s^2}{1 + c_5\, r_s + c_6\, r_s^2 + c_7\, r_s^3}, \tag{12}$$

$$\tag{13}$$

$$\mu_{rev}(r_s) = \frac{\pi^2}{3}\,\beta_{rev}\left(r_s\right), \tag{14}$$

$$\mu_{mod/HL}(r_s) = \frac{\pi^2}{3}\,\beta_{mod/HL}\left(r_s\right), \tag{15}$$

$$\mu_{RG}(r_s) = \frac{16\,\pi^2}{3}\left(\frac{3}{\pi}\right)^{1/3} C_{RG}(r_s). \tag{16}$$

Each Padé approximant evidently has its own set of parameters $\{c_n\}$. See the main text for other details.

III. TABULATIONS OF TEST SET RESULTS

The tables that follow tabulate mean absolute deviations, MAD, mean deviations, MD, and mean absolute relative deviations, MARD, from the eight locally-parametrized functionals presented in the main text for the various molecular and solid test sets.

Table I. Deviations for standard enthalpies of formation from the G3/99 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	21.21 ± 1.00	29.97 ± 1.31	29.14 ± 1.28	26.84 ± 1.19	25.89 ± 1.16
		MD	-20.69 ± 1.04	-29.71 ± 1.34	-28.87 ± 1.31	-26.52 ± 1.23	-25.54 ± 1.19
	P86	MAD	41.58 ± 1.70	46.52 ± 1.91	45.01 ± 1.85	47.93 ± 1.98	46.71 ± 1.93
		MD	-41.55 ± 1.70	-46.50 ± 1.91	-44.98 ± 1.85	-47.90 ± 1.98	-46.68 ± 1.93
*lp*lsRPBE	PBE	MAD	7.93 ± 0.43	11.79 ± 0.62	12.60 ± 0.63	10.44 ± 0.58	8.36 ± 0.48
		MD	-1.09 ± 0.68	-10.85 ± 0.70	9.45 ± 0.84	6.85 ± 0.79	-5.53 ± 0.64
	P86	MAD	22.31 ± 0.86	27.87 ± 1.10	11.16 ± 0.50	16.15 ± 0.66	26.92 ± 1.07
		MD	-22.01 ± 0.89	-27.71 ± 1.12	-6.74 ± 0.78	-14.61 ± 0.81	-26.74 ± 1.09
*lp*CAP	PBE	MAD	9.23 ± 0.49	21.30 ± 0.95	20.55 ± 0.92	15.97 ± 0.78	16.08 ± 0.78
		MD	-0.35 ± 0.79	-20.71 ± 1.01	-19.94 ± 0.98	-15.12 ± 0.85	-15.27 ± 0.85
	P86	MAD	21.53 ± 0.80	37.52 ± 1.49	36.08 ± 1.43	36.54 ± 1.45	35.46 ± 1.45
		MD	-21.09 ± 0.85	-37.40 ± 1.50	-35.96 ± 1.44	-36.41 ± 1.47	-36.32 ± 1.47
*lp*NCAP	PBE	MAD	19.94 ± 1.10	28.24 ± 1.29	26.42 ± 1.26	24.86 ± 1.25	24.35 ± 1.24
		MD	18.24 ± 1.23	27.20 ± 1.39	25.37 ± 1.35	23.75 ± 1.35	23.21 ± 1.34
	P86	MAD	5.97 ± 0.35	13.58 ± 0.74	12.33 ± 0.62	7.14 ± 0.44	6.94 ± 0.42
		MD	-2.70 ± 0.50	10.33 ± 0.95	9.17 ± 0.83	2.29 ± 0.63	1.99 ± 0.61

Table II. Mean absolute deviations per atom, in kcal/mol, for standard enthalpies of formation from the G3/99 set.

X	C	μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	3.19	4.19	4.08	3.82	3.71
	P86	5.46	6.02	5.85	6.18	6.05
*lp*lsRPBE	PBE	1.43	2.02	2.01	1.64	1.57
	P86	3.12	3.74	1.97	2.36	3.64
*lp*CAP	PBE	1.62	3.22	3.12	2.59	2.59
	P86	3.14	4.98	4.81	4.85	4.84
*lp*NCAP	PBE	2.33	3.76	3.36	3.01	2.93
	P86	1.27	2.39	2.04	1.43	1.38

Table III. Mean absolute deviations per electron, in kcal/mol, for standard enthalpies of formation from the G3/99 set.

X	C	μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	0.63	0.86	0.84	0.78	0.75
	P86	1.22	1.36	1.31	1.39	1.36
*lp*lsRPBE	PBE	0.26	0.37	0.40	0.35	0.28
	P86	0.69	0.85	0.38	0.52	0.82
*lp*CAP	PBE	0.30	0.63	0.60	0.48	0.49
	P86	0.67	1.11	1.06	1.07	1.07
*lp*NCAP	PBE	0.58	0.79	0.75	0.71	0.70
	P86	0.23	0.40	0.36	0.25	0.24

Table IV. Deviations for adiabatic ionization potentials from the IP13/3 set employing the 6-31++G(d,p) basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	3.47 ± 0.85	3.19 ± 0.80	3.18 ± 0.80	3.24 ± 0.82	3.24 ± 0.82
		MD	2.77 ± 1.03	2.39 ± 1.00	2.34 ± 1.01	2.43 ± 1.02	2.43 ± 1.03
		MARD	1.32 ± 1.74	1.21 ± 1.06	1.20 ± 1.07	1.23 ± 1.08	1.23 ± 1.09
	P86	MAD	5.60 ± 1.06	4.75 ± 1.01	4.83 ± 1.02	4.82 ± 1.02	5.00 ± 1.02
		MD	5.38 ± 1.15	4.40 ± 1.14	4.49 ± 1.15	4.48 ± 1.14	4.68 ± 1.15
		MARD	2.14 ± 1.48	1.79 ± 1.36	1.82 ± 1.38	1.82 ± 1.38	1.90 ± 1.40
*lp*lsRPBE	PBE	MAD	3.30 ± 0.78	2.96 ± 0.69	4.73 ± 1.41	4.11 ± 1.04	3.06 ± 0.74
		MD	2.59 ± 0.98	1.96 ± 0.95	1.97 ± 1.88	2.28 ± 1.43	2.07 ± 0.98
		MARD	1.27 ± 1.05	1.13 ± 0.98	1.84 ± 1.88	1.59 ± 1.45	1.16 ± 1.02
	P86	MAD	5.40 ± 1.00	4.34 ± 0.93	6.38 ± 1.30	5.68 ± 1.04	4.65 ± 0.96
		MD	5.21 ± 1.08	3.98 ± 1.06	4.12 ± 1.92	4.32 ± 1.49	4.32 ± 1.08
		MARD	2.08 ± 1.41	1.65 ± 1.26	2.46 ± 1.98	2.18 ± 1.61	1.77 ± 1.31
*lp*CAP	PBE	MAD	2.55 ± 0.53	2.47 ± 0.50	2.50 ± 0.52	2.52 ± 0.52	2.55 ± 0.54
		MD	-0.88 ± 0.87	-0.78 ± 0.84	-0.91 ± 0.85	-0.98 ± 0.85	-1.12 ± 0.86
		MARD	0.98 ± 1.02	0.96 ± 0.98	0.97 ± 1.01	0.97 ± 1.02	0.98 ± 1.05
	P86	MAD	2.65 ± 0.62	2.39 ± 0.59	2.39 ± 0.59	2.36 ± 0.57	2.38 ± 0.58
		MD	1.73 ± 0.85	1.24 ± 0.84	1.24 ± 0.83	1.08 ± 0.83	1.13 ± 0.84
		MARD	1.01 ± 0.87	0.90 ± 0.84	0.90 ± 0.84	0.89 ± 0.84	0.90 ± 0.84
*lp*NCAP	PBE	MAD	2.84 ± 0.62	4.89 ± 1.80	4.26 ± 1.35	3.67 ± 0.96	3.55 ± 0.90
		MD	0.94 ± 0.99	0.27 ± 2.29	0.56 ± 1.82	0.78 ± 1.41	0.78 ± 1.35
		MARD	1.07 ± 2.93	1.89 ± 2.33	1.64 ± 1.85	1.41 ± 1.43	1.36 ± 1.36
	P86	MAD	4.00 ± 0.92	5.70 ± 1.73	5.16 ± 1.34	4.46 ± 1.06	4.47 ± 1.02
		MD	3.55 ± 1.06	2.29 ± 2.29	2.70 ± 1.84	2.82 ± 1.46	3.02 ± 1.39
		MARD	1.52 ± 1.21	2.18 ± 2.29	1.97 ± 1.86	1.70 ± 1.49	1.70 ± 1.44

Table V. Deviations for adiabatic electron affinities from the EA13/3 set employing the 6-31++G(d,p) basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	2.64 ± 0.98	2.54 ± 0.90	2.48 ± 0.90	2.49 ± 0.92	2.46 ± 0.92
		MD	2.37 ± 1.03	2.13 ± 0.99	0.99 ± 0.99	2.08 ± 1.00	1.99 ± 1.01
		MARD	7.20 ± 1.74	7.23 ± 1.77	1.76 ± 1.76	7.02 ± 1.74	6.94 ± 1.75
	P86	MAD	6.29 ± 0.99	4.87 ± 0.96	4.91 ± 0.97	4.93 ± 0.97	5.22 ± 0.97
		MD	6.29 ± 0.99	4.87 ± 0.96	4.91 ± 0.97	4.93 ± 0.97	5.22 ± 0.97
		MARD	19.81 ± 4.03	14.94 ± 3.06	15.11 ± 3.10	15.15 ± 3.10	16.13 ± 3.30
*lp*lsRPBE	PBE	MAD	2.60 ± 1.05	2.41 ± 0.93	5.52 ± 1.92	4.26 ± 1.47	2.42 ± 0.95
		MD	2.25 ± 1.11	1.67 ± 1.05	0.87 ± 2.49	1.25 ± 1.88	1.54 ± 1.09
		MARD	7.04 ± 1.78	6.95 ± 1.85	13.36 ± 4.38	10.77 ± 3.33	6.84 ± 1.88
	P86	MAD	6.17 ± 1.08	4.42 ± 1.03	6.54 ± 1.94	5.27 ± 1.59	4.76 ± 1.05
		MD	6.17 ± 1.08	4.42 ± 1.03	3.75 ± 2.48	4.12 ± 1.86	4.76 ± 1.05
		MARD	19.49 ± 3.99	13.50 ± 2.82	19.08 ± 5.07	16.48 ± 4.02	14.72 ± 3.06
*lp*CAP	PBE	MAD	3.65 ± 0.56	3.18 ± 0.54	3.27 ± 0.54	3.52 ± 0.53	3.57 ± 0.53
		MD	-1.94 ± 1.05	-1.35 ± 0.99	-1.47 ± 1.00	-1.67 ± 1.01	-1.90 ± 1.02
		MARD	13.39 ± 4.55	12.03 ± 3.99	12.33 ± 4.11	12.80 ± 4.30	13.32 ± 4.51
	P86	MAD	2.59 ± 0.81	2.36 ± 0.71	2.36 ± 0.72	2.38 ± 0.69	2.39 ± 0.71
		MD	1.91 ± 0.95	1.34 ± 0.91	1.37 ± 0.91	1.13 ± 0.92	1.29 ± 0.92
		MARD	8.36 ± 2.09	7.86 ± 2.09	7.84 ± 2.08	8.07 ± 2.20	8.01 ± 2.15
*lp*NCAP	PBE	MAD	2.92 ± 0.77	6.82 ± 2.24	5.73 ± 1.78	4.64 ± 1.32	4.47 ± 1.25
		MD	-0.25 ± 1.14	-1.33 ± 2.96	-1.16 ± 2.40	-0.93 ± 1.86	-0.91 ± 1.78
		MARD	9.08 ± 2.93	17.02 ± 6.07	14.81 ± 5.20	12.64 ± 4.34	12.32 ± 4.21
	P86	MAD	3.70 ± 1.05	6.64 ± 2.27	5.60 ± 1.82	4.41 ± 1.41	4.36 ± 1.36
		MD	3.62 ± 1.08	1.36 ± 2.95	1.68 ± 2.38	1.87 ± 1.82	2.28 ± 1.73
		MARD	11.17 ± 2.43	16.34 ± 5.23	14.48 ± 4.40	11.91 ± 3.42	12.21 ± 3.35

Table VI. Deviations for proton affinities from the PA8 set employing the 6-31++G(d,p) basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	1.39 ± 0.32	1.59 ± 0.29	1.50 ± 0.31	1.44 ± 0.31	1.37 ± 0.32
		MD	-0.73 ± 0.55	-0.99 ± 0.56	-0.86 ± 0.55	-0.79 ± 0.55	-0.70 ± 0.55
		MARD	1.00 ± 0.35	1.12 ± 0.34	1.00 ± 0.36	1.00 ± 0.35	0.88 ± 0.37
	P86	MAD	2.28 ± 0.31	1.78 ± 0.26	1.86 ± 0.26	1.96 ± 0.26	2.13 ± 0.28
		MD	-1.95 ± 0.54	-1.27 ± 0.54	-1.36 ± 0.54	-1.50 ± 0.54	-1.74 ± 0.54
		MARD	1.38 ± 0.46	1.00 ± 0.40	1.12 ± 0.38	1.12 ± 0.41	1.38 ± 0.40
*lp*lsRPBE	PBE	MAD	1.22 ± 0.37	1.12 ± 0.40	1.14 ± 0.40	1.17 ± 0.39	1.19 ± 0.39
		MD	0.07 ± 0.59	-0.07 ± 0.58	0.10 ± 0.58	0.14 ± 0.59	0.24 ± 0.59
		MARD	0.62 ± 0.44	0.50 ± 0.46	0.50 ± 0.46	0.50 ± 0.46	0.62 ± 0.45
	P86	MAD	1.71 ± 0.35	1.27 ± 0.36	1.29 ± 0.36	1.32 ± 0.37	1.46 ± 0.36
		MD	-1.16 ± 0.59	-0.36 ± 0.58	-0.40 ± 0.59	-0.57 ± 0.58	-0.81 ± 0.58
		MARD	0.88 ± 0.47	0.75 ± 0.41	0.75 ± 0.41	0.75 ± 0.43	0.88 ± 0.42
*lp*CAP	PBE	MAD	1.53 ± 0.53	1.14 ± 0.47	1.18 ± 0.46	1.27 ± 0.47	1.35 ± 0.48
		MD	1.37 ± 0.59	0.35 ± 0.62	0.49 ± 0.62	0.75 ± 0.61	0.95 ± 0.60
		MARD	0.88 ± 0.58	0.75 ± 0.49	0.75 ± 0.49	0.88 ± 0.49	0.88 ± 0.51
	P86	MAD	0.93 ± 0.46	0.95 ± 0.47	0.98 ± 0.46	0.96 ± 0.47	1.01 ± 0.45
		MD	0.17 ± 0.58	0.07 ± 0.59	-0.02 ± 0.59	0.05 ± 0.60	-0.08 ± 0.59
		MARD	0.38 ± 0.51	0.50 ± 0.50	0.50 ± 0.49	0.50 ± 0.50	0.50 ± 0.49
*lp*NCAP	PBE	MAD	2.38 ± 0.58	1.91 ± 0.56	2.05 ± 0.56	2.17 ± 0.57	2.31 ± 0.57
		MD	2.38 ± 0.58	1.91 ± 0.56	2.05 ± 0.56	2.17 ± 0.57	2.31 ± 0.57
		MARD	1.62 ± 0.64	1.00 ± 0.66	1.25 ± 0.64	1.38 ± 0.64	1.50 ± 0.65
	P86	MAD	1.32 ± 0.52	1.63 ± 0.56	1.54 ± 0.56	1.47 ± 0.56	1.36 ± 0.53
		MD	1.18 ± 0.56	1.63 ± 0.56	1.54 ± 0.56	1.47 ± 0.56	1.28 ± 0.56
		MARD	0.75 ± 0.56	0.88 ± 0.63	0.88 ± 0.62	0.88 ± 0.60	0.75 ± 0.58

Table VII. Deviations for bond lengths from the T96-R1 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	0.0163 ± 0.001	0.0154 ± 0.001	0.0154 ± 0.001	0.0156 ± 0.001	0.0157 ± 0.001
		MD	0.0161 ± 0.001	0.0151 ± 0.001	0.0151 ± 0.001	0.0154 ± 0.001	0.0155 ± 0.001
		MARD	1.067 ± 0.108	1.013 ± 0.102	1.011 ± 0.102	1.024 ± 0.103	1.029 ± 0.104
	P86	MAD	0.0171 ± 0.001	0.0169 ± 0.001	0.0169 ± 0.001	0.0166 ± 0.001	0.0160 ± 0.001
		MD	0.0169 ± 0.001	0.0152 ± 0.001	0.0151 ± 0.001	0.0147 ± 0.001	0.0156 ± 0.001
		MARD	1.126 ± 0.114	1.108 ± 0.112	1.108 ± 0.112	1.089 ± 0.110	1.054 ± 0.107
*lp*lsRPBE	PBE	MAD	0.0219 ± 0.001	0.0205 ± 0.001	0.0210 ± 0.001	0.0213 ± 0.001	0.0211 ± 0.001
		MD	0.0219 ± 0.001	0.0204 ± 0.001	0.0210 ± 0.001	0.0213 ± 0.001	0.0210 ± 0.001
		MARD	1.386 ± 0.140	1.302 ± 0.131	1.334 ± 0.135	1.349 ± 0.136	1.336 ± 0.135
	P86	MAD	0.0223 ± 0.001	0.0214 ± 0.001	0.0219 ± 0.001	0.0214 ± 0.001	0.0208 ± 0.001
		MD	0.0223 ± 0.001	0.0214 ± 0.001	0.0219 ± 0.001	0.0214 ± 0.001	0.0208 ± 0.001
		MARD	1.436 ± 0.145	1.377 ± 0.139	1.409 ± 0.142	1.384 ± 0.140	1.345 ± 0.136
*lp*CAP	PBE	MAD	0.0205 ± 0.002	0.0182 ± 0.001	0.0184 ± 0.001	0.0190 ± 0.002	0.0191 ± 0.002
		MD	0.0201 ± 0.002	0.0174 ± 0.002	0.0177 ± 0.002	0.0184 ± 0.002	0.0184 ± 0.002
		MARD	1.272 ± 0.128	1.151 ± 0.116	1.164 ± 0.118	1.195 ± 0.121	1.195 ± 0.121
	P86	MAD	0.0207 ± 0.001	0.0188 ± 0.001	0.0190 ± 0.001	0.0189 ± 0.001	0.0186 ± 0.001
		MD	0.0204 ± 0.001	0.0183 ± 0.001	0.0186 ± 0.001	0.0184 ± 0.001	0.0181 ± 0.001
		MARD	1.305 ± 0.132	1.207 ± 0.122	1.222 ± 0.123	1.214 ± 0.123	1.192 ± 0.120
*lp*NCAP	PBE	MAD	0.0232 ± 0.002	0.0218 ± 0.001	0.0220 ± 0.001	0.0223 ± 0.001	0.0224 ± 0.001
		MD	0.0231 ± 0.002	0.0217 ± 0.001	0.0219 ± 0.001	0.0223 ± 0.001	0.0224 ± 0.001
		MARD	1.428 ± 0.144	1.350 ± 0.136	1.362 ± 0.137	1.380 ± 0.139	1.387 ± 0.140
	P86	MAD	0.0236 ± 0.001	0.0227 ± 0.001	0.0229 ± 0.001	0.0224 ± 0.001	0.0222 ± 0.001
		MD	0.0236 ± 0.001	0.0227 ± 0.001	0.0229 ± 0.001	0.0224 ± 0.001	0.0222 ± 0.001
		MARD	1.477 ± 0.149	1.427 ± 0.144	1.438 ± 0.145	1.413 ± 0.143	1.396 ± 0.141

Table VIII. Deviations for weak interactions from the HB6/04, CT7/04, DI6/04, WI7/05 and PPS5/05 sets employing the 6-31++G(d,p) basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	1.64 ± 0.34	1.79 ± 0.35	1.79 ± 0.35	1.74 ± 0.35	1.73 ± 0.35
		MD	0.80 ± 0.43	1.04 ± 0.44	1.04 ± 0.44	0.98 ± 0.44	0.97 ± 0.43
		MARD	108.17±19.45	107.37±19.28	106.28±19.08	106.52± 19.13	106.12±19.06
	P86	MAD	2.04 ± 0.37	2.03 ± 0.37	1.99 ± 0.37	2.16 ± 0.39	2.12 ± 0.38
		MD	1.46 ± 0.45	1.49 ± 0.45	1.39 ± 0.45	1.69 ± 0.46	1.57 ± 0.46
		MARD	111.58±20.00	107.28±19.22	104.92±18.80	112.64±20.17	107.40±19.22
*lp*lsRPBE	PBE	MAD	1.53 ± 0.29	1.55 ± 0.31	1.55 ± 0.31	1.54 ± 0.30	1.53 ± 0.30
		MD	0.42 ± 0.40	0.49 ± 0.41	0.47 ± 0.41	0.43 ± 0.41	0.37 ± 0.40
		MARD	156.98±28.38	141.24±25.51	138.95±25.09	143.55±25.93	140.77±25.42
	P86	MAD	1.73 ± 0.32	1.65 ± 0.32	1.62 ± 0.32	1.75 ± 0.33	1.70 ± 0.33
		MD	1.07 ± 0.41	0.93 ± 0.41	0.82 ± 0.41	1.14 ± 0.41	0.96 ± 0.42
		MARD	162.12±29.28	141.52±25.54	137.31±24.78	148.74±26.84	139.98±25.25
*lp*CAP	PBE	MAD	2.70 ± 0.42	1.85 ± 0.36	1.82 ± 0.36	1.91 ± 0.37	1.83 ± 0.35
		MD	-2.25 ± 0.50	-0.81 ± 0.47	-0.72 ± 0.47	-1.04 ± 0.47	-0.87 ± 0.46
		MARD	255.95±46.24	169.63±30.63	162.01±29.25	176.27±31.83	155.97±28.14
	P86	MAD	2.28 ± 0.40	1.76 ± 0.35	1.76 ± 0.35	1.75 ± 0.35	1.74 ± 0.36
		MD	-1.63 ± 0.50	-0.39 ± 0.47	-0.40 ± 0.47	-0.36 ± 0.47	-0.29 ± 0.47
		MARD	245.45±44.40	165.77±29.95	163.12±29.46	167.64±30.29	155.96±28.16
*lp*NCAP	PBE	MAD	2.84 ± 0.42	2.46 ± 0.39	2.45 ± 0.39	2.53 ± 0.39	2.52 ± 0.39
		MD	-2.51 ± 0.49	-1.98 ± 0.47	-1.96 ± 0.47	-2.08 ± 0.47	-2.07 ± 0.47
		MARD	262.20±47.35	244.43±44.14	241.57±43.66	246.39±44.52	243.19±43.94
	P86	MAD	2.39 ± 0.39	2.16 ± 0.37	2.21 ± 0.38	2.07 ± 0.36	2.14 ± 0.37
		MD	-1.89 ± 0.47	-1.57 ± 0.46	-1.64 ± 0.46	-1.42 ± 0.46	-1.50 ± 0.47
		MARD	250.46± 45.29	233.70±42.28	237.69±42.99	229.70±41.56	235.55±42.62

Table IX. Deviations of forward non-hydrogen transfer barrier heights from the NHTBH38/04 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	10.38 ± 1.67	10.80 ± 1.63	10.78 ± 1.64	10.67 ± 1.65	10.62 ± 1.65
		MD	-6.62 ± 2.51	-7.10 ± 2.52	-7.07 ± 2.52	-6.95 ± 2.52	-6.98 ± 2.52
		MARD	410.98 ±94.44	423.92 ±97.39	424.57 ±97.54	421.22 ±96.78	149.87 ±96.48
	P86	MAD	12.01 ± 1.49	11.96 ± 1.50	11.88 ± 1.51	12.17 ± 1.50	12.17 ± 1.48
		MD	-8.64 ± 2.46	-8.53 ± 2.48	-8.45 ± 2.48	-8.76 ± 2.49	-8.80 ± 2.48
		MARD	456.44 ±104.76	454.19 ±104.24	451.30 ±103.58	463.42 ±106.37	462.76 ±106.22
*lp*lsRPBE	PBE	MAD	9.76 ± 1.71	10.14 ± 1.67	13.58 ± 1.40	12.44 ± 1.37	9.90 ± 1.69
		MD	-5.97 ± 2.49	-6.38 ± 2.49	-10.74 ± 2.41	-9.31 ± 2.38	-6.11 ± 2.50
		MARD	391.41 ±89.97	400.53 ±92.03	443.50 ±101.34	429.89 ±98.40	394.77 ± 90.73
	P86	MAD	11.39 ± 1.51	11.31 ± 1.53	14.69 ± 1.45	13.95 ± 1.36	11.45 ± 1.51
		MD	-7.99 ± 2.44	-7.82 ± 2.46	-12.13 ± 2.44	-11.13 ± 2.40	-8.03 ± 2.45
		MARD	473.01 ±100.33	430.96 ±98.93	470.45 ±107.43	472.28 ±108.04	437.60 ±100.46
*lp*CAP	PBE	MAD	8.22 ± 1.79	9.62 ± 1.67	9.66 ± 1.67	9.34 ± 1.70	9.37 ± 1.70
		MD	-4.20 ± 2.45	-5.74 ± 2.47	-5.77 ± 2.48	-5.42 ± 2.47	-5.44 ± 2.48
		MARD	292.69 ±67.07	352.47 ±80.83	356.10 ±81.67	342.79 ±78.61	345.20 ±79.18
	P86	MAD	9.83 ± 1.57	10.76 ± 1.52	10.74 ± 1.53	10.83 ± 1.52	10.90 ± 1.50
		MD	-6.19 ± 2.39	-7.15 ± 2.43	-7.13 ± 2.43	-7.22 ± 2.44	-7.33 ± 2.43
		MARD	337.71 ±77.30	382.23 ±87.57	382.37 ±87.61	384.53 ±88.10	387.75 ± 88.84
*lp*NCAP	PBE	MAD	7.78 ± 1.83	12.58 ± 1.49	11.72 ± 1.41	10.63 ± 1.43	10.22 ± 1.47
		MD	-3.74 ± 2.44	-9.78 ± 2.38	-8.63 ± 2.34	-7.27 ± 2.32	-6.73 ± 2.33
		MARD	286.35 ±65.68	357.98 ±81.43	352.61 ± 80.36	337.38 ±77.03	331.77 ±75.81
	P86	MAD	9.39 ± 1.60	13.73 ± 1.54	12.82 ± 1.41	12.12 ± 1.36	11.75 ± 1.36
		MD	-5.74 ± 2.37	-11.21 ± 2.42	-10.01 ± 2.36	-9.07 ± 2.33	-8.63 ± 2.32
		MARD	331.32 ±75.90	387.96 ±88.22	379.14 ±86.36	379.12 ±86.51	374.33 ±85.47

Table X. Deviations of reverse non-hydrogen transfer barrier heights from the NHTBH38/04 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	9.96 ± 1.78	10.24 ± 1.85	10.23 ± 1.84	10.16 ± 1.82	10.13 ± 1.81
		MD	-7.72 ± 2.32	-8.05 ± 2.38	-8.03 ± 2.37	-7.94 ± 2.36	-7.89 ± 2.35
		MARD	262.17 ±59.47	270.96 ±61.48	271.64 ±61.64	269.40 ±61.13	268.47 ±60.92
	P86	MAD	10.93 ± 1.85	10.87 ± 1.85	10.82 ± 1.84	11.05 ± 1.88	11.04 ± 1.89
		MD	-8.88 ± 2.38	-8.68 ± 2.41	-8.64 ± 2.40	-8.90 ± 2.43	-8.97 ± 2.42
		MARD	295.39 ±67.07	291.95 ±66.28	290.03 ±65.84	299.52 ±68.02	299.58 ±68.04
*lp*lsRPBE	PBE	MAD	9.44 ± 1.62	9.67 ± 1.68	11.14 ± 2.09	10.61 ± 1.93	9.52 ± 1.64
		MD	-6.98 ± 2.21	-7.26 ± 2.26	-9.24 ± 2.56	-8.53 ± 2.43	-7.05 ± 2.23
		MARD	248.71 ±56.42	253.86 ±57.58	258.19 ±58.27	254.97 ±57.63	250.22 ±56.76
	P86	MAD	10.41 ± 1.67	10.32 ± 1.68	11.74 ± 2.12	11.50 ± 2.01	10.44 ± 1.69
		MD	-8.15 ± 2.26	-7.89 ± 2.29	-9.86 ± 2.60	-9.49 ± 2.53	-8.13 ± 2.29
		MARD	281.94 ±64.02	274.89 ±62.38	276.61 ±62.47	285.12 ±64.52	281.18 ±63.84
*lp*CAP	PBE	MAD	7.99 ± 1.71	9.08 ± 1.83	9.12 ± 1.82	8.88 ± 1.79	8.90 ± 1.78
		MD	-5.21 ± 2.23	-6.57 ± 2.35	-6.59 ± 2.35	-6.28 ± 2.32	-6.28 ± 2.32
		MARD	160.17 ±35.91	207.35 ±46.77	210.39 ±47.47	199.89 ±45.06	201.74 ±45.49
	P86	MAD	8.95 ± 1.71	9.71 ± 1.80	9.71 ± 1.80	9.75 ± 1.81	9.81 ± 1.81
		MD	-6.36 ± 2.26	-7.19 ± 2.37	-7.19 ± 2.37	-7.22 ± 2.38	-7.35 ± 2.37
		MARD	193.00 ±43.42	227.97 ±51.48	228.42 ±51.58	229.65 ±51.86	232.50 ±52.52
*lp*NCAP	PBE	MAD	7.75 ± 1.56	10.04 ± 2.02	9.64 ± 1.88	9.10 ± 1.76	8.91 ± 1.71
		MD	-4.77 ± 2.12	-7.80 ± 2.51	-7.25 ± 2.40	-6.55 ± 2.31	-6.28 ± 2.27
		MARD	159.07 ±35.70	182.83 ±40.78	182.76 ±40.85	177.19 ±39.66	175.92 ±39.40
	P86	MAD	8.71 ± 1.53	10.67 ± 2.03	10.23 ± 1.89	9.98 ± 1.80	9.83 ± 1.74
		MD	-5.92 ± 2.14	-8.42 ± 2.55	-7.86 ± 2.44	-7.49 ± 2.38	-7.36 ± 2.32
		MARD	191.94 ±43.21	203.48 ±45.49	200.82 ±44.96	206.81 ±46.43	206.68 ±46.43

Table XI. Deviations of forward hydrogen transfer barrier heights from the HTBH38/04 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	9.49 ± 0.96	10.31 ± 0.99	10.20 ± 0.98	9.98 ± 0.98	9.89 ± 0.97
		MD	-9.49 ± 0.96	-10.31 ± 0.99	-10.20 ± 0.98	-9.98 ± 0.98	-9.89 ± 0.97
		MARD	190.90 ±42.77	206.47 ±46.25	204.37 ±45.78	200.30 ±44.87	198.47 ±44.46
	P86	MAD	11.30 ± 0.95	11.40 ± 0.94	11.30 ± 0.94	11.67 ± 0.96	11.64 ± 0.96
		MD	-11.30 ± 0.95	-11.40 ± 0.94	-11.30 ± 0.94	-11.67 ± 0.96	-11.64 ± 0.96
		MARD	227.56 ±50.98	229.42 ±51.40	227.19 ±50.90	234.65 ±52.57	233.94 ±52.41
*lp*lsRPBE	PBE	MAD	7.76 ± 0.81	8.58 ± 0.83	12.82 ± 1.26	11.27 ± 1.09	8.03 ± 0.81
		MD	-7.76 ± 0.81	-8.58 ± 0.83	-12.82 ± 1.26	-11.27 ± 1.09	-8.03 ± 0.81
		MARD	156.63 ±35.10	171.83 ±38.49	269.91 ±60.61	232.56 ±52.17	161.45 ±36.17
	P86	MAD	9.58 ± 0.84	9.68 ± 0.82	13.94 ± 1.30	12.97 ± 1.13	9.78 ± 0.83
		MD	-9.58 ± 0.84	-9.68 ± 0.82	-13.94 ± 1.30	-12.97 ± 1.13	-9.78 ± 0.83
		MARD	193.34 ±43.32	194.94 ±43.67	293.01 ±65.79	267.16 ±59.92	196.93 ±44.12
*lp*CAP	PBE	MAD	6.92 ± 0.76	9.17 ± 0.86	9.13 ± 0.85	8.60 ± 0.82	8.62 ± 0.82
		MD	-6.92 ± 0.76	-9.17 ± 0.86	-9.13 ± 0.85	-8.60 ± 0.82	-8.62 ± 0.82
		MARD	135.45 ±30.30	180.38 ±40.36	179.44 ±40.15	169.02 ±37.82	169.53 ±37.94
	P86	MAD	8.70 ± 0.77	10.25 ± 0.81	10.20 ± 0.81	10.27 ± 0.80	10.35 ± 0.81
		MD	-8.70 ± 0.77	-10.25 ± 0.81	-10.20 ± 0.81	-10.27 ± 0.80	-10.35 ± 0.81
		MARD	171.64 ±38.41	202.95 ±45.43	201.88 ±45.19	202.97 ±45.43	204.69 ±45.81
*lp*NCAP	PBE	MAD	5.04 ± 0.68	11.16 ± 1.29	10.21 ± 1.12	8.73 ± 0.96	8.21 ± 0.90
		MD	-5.00 ± 0.69	-11.16 ± 1.29	-10.21 ± 1.12	-8.73 ± 0.96	-8.21 ± 0.90
		MARD	100.39 ±22.49	240.75 ±54.13	215.81 ±48.47	180.39 ±40.47	169.43 ±38.01
	P86	MAD	6.80 ± 0.75	12.25 ± 1.36	11.31 ± 1.18	10.41 ± 1.01	9.95 ± 0.96
		MD	-6.80 ± 0.75	-12.25 ± 1.36	-11.31 ± 1.18	-10.41 ± 1.01	-9.95 ± 0.96
		MARD	136.36 ±30.55	263.71 ±59.28	238.53 ±53.57	214.53 ±48.12	204.71 ±45.91

Table XII. Deviations of reverse hydrogen transfer barrier heights from the HTBH38/04 set employing the Def2-TZVPP basis set.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	9.72 ± 0.73	10.50 ± 0.76	10.42 ± 0.76	10.22 ± 0.75	10.13 ± 0.75
		MD	-9.72 ± 0.73	-10.50 ± 0.76	-10.42 ± 0.76	-10.22 ± 0.75	-10.13 ± 0.75
		MARD	68.78 ±13.94	74.40 ±15.08	73.77 ±14.95	72.33 ±14.66	71.66 ±14.52
	P86	MAD	11.30 ± 0.75	11.42 ± 0.75	11.32 ± 0.75	11.70 ± 0.75	11.65 ± 0.75
		MD	-11.30 ± 0.75	-11.42 ± 0.75	-11.32 ± 0.75	-11.70 ± 0.75	-11.65 ± 0.75
		MARD	79.32 ±16.05	80.20 ±16.23	79.48 ±16.08	82.17 ±16.63	81.83 ±16.56
*lp*lsRPBE	PBE	MAD	8.25 ± 0.69	9.01 ± 0.69	12.58 ± 0.97	11.51 ± 0.86	8.52 ± 0.68
		MD	-8.25 ± 0.69	-9.01 ± 0.69	-12.58 ± 0.97	-11.51 ± 0.86	-8.52 ± 0.68
		MARD	57.69 ±11.67	63.23 ±12.80	84.97 ±17.09	78.30 ±15.77	59.62 ±12.06
	P86	MAD	9.84 ± 0.77	9.94 ± 0.76	13.50 ± 1.09	13.00 ± 0.98	10.05 ± 0.75
		MD	-9.84 ± 0.77	-9.94 ± 0.76	-13.50 ± 1.09	-13.00 ± 0.98	-10.05 ± 0.75
		MARD	68.25 ±13.79	69.11 ±13.97	90.79 ±18.25	88.20 ±17.75	69.83 ±14.11
*lp*CAP	PBE	MAD	7.11 ± 0.63	9.33 ± 0.70	9.32 ± 0.70	8.82 ± 0.67	8.85 ± 0.67
		MD	-7.11 ± 0.63	-9.33 ± 0.70	-9.32 ± 0.70	-8.82 ± 0.67	-8.85 ± 0.67
		MARD	50.57 ±10.26	66.59 ±13.52	66.50 ±13.50	62.88 ±12.76	63.10 ±12.80
	P86	MAD	8.66 ± 0.67	10.23 ± 0.68	10.21 ± 0.68	10.27 ± 0.68	10.36 ± 0.68
		MD	-8.66 ± 0.67	-10.23 ± 0.68	-10.21 ± 0.68	-10.27 ± 0.68	-10.36 ± 0.68
		MARD	60.92 ±12.34	72.25 ±14.63	72.08 ±14.60	72.56 ±14.70	73.15 ±14.82
*lp*NCAP	PBE	MAD	5.45 ± 0.61	10.38 ± 0.96	9.96 ± 0.87	8.92 ± 0.78	8.41 ± 0.73
		MD	-5.40 ± 0.63	-10.38 ± 0.96	-9.96 ± 0.87	-8.92 ± 0.78	-8.41 ± 0.73
		MARD	37.67 ± 7.62	68.97 ±13.84	66.61 ±13.38	60.03 ±12.07	56.76 ±11.42
	P86	MAD	6.98 ± 0.76	11.30 ± 1.13	10.86 ± 1.04	10.39 ± 0.93	9.92 ± 0.87
		MD	-6.96 ± 0.76	-11.30 ± 1.13	-10.86 ± 1.04	-10.39 ± 0.93	-9.92 ± 0.87
		MARD	47.95 ± 9.69	74.74 ±15.00	72.28 ±14.51	69.79 ±14.03	66.86 ±13.45

Table XIII. Deviations for lattice constants of 54 solids bounded by strong interactions.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	0.053 ± 0.006	0.043 ± 0.005	0.044 ± 0.005	0.046 ± 0.005	0.047 ± 0.005
		MD	0.047 ± 0.007	0.035 ± 0.006	0.036 ± 0.006	0.039 ± 0.006	0.041 ± 0.006
		MARD	1.122 ± 0.147	0.913 ± 0.120	0.941 ± 0.123	0.991 ± 0.130	0.998 ± 0.131
*lp*lsRPBE	PBE	MAD	0.089 ± 0.010	0.072 ± 0.008	0.073 ± 0.008	0.078 ± 0.008	0.081 ± 0.008
		MD	0.089 ± 0.010	0.071 ± 0.008	0.073 ± 0.008	0.078 ± 0.009	0.080 ± 0.009
		MARD	1.887 ± 0.247	1.515 ± 0.198	1.556 ± 0.204	1.651 ± 0.216	1.721 ± 0.225
*lp*CAP	PBE	MAD	0.057 ± 0.010	0.041 ± 0.005	0.041 ± 0.005	0.045 ± 0.006	0.047 ± 0.007
		MD	0.052 ± 0.010	0.026 ± 0.007	0.029 ± 0.007	0.034 ± 0.008	0.037 ± 0.008
		MARD	1.182 ± 0.155	0.883 ± 0.116	0.878 ± 0.115	0.956 ± 0.125	0.983 ± 0.129
*lp*NCAP	P86	MAD	0.083 ± 0.009	0.076 ± 0.008	0.076 ± 0.008	0.073 ± 0.008	0.071 ± 0.008
		MD	0.082 ± 0.009	0.075 ± 0.008	0.074 ± 0.008	0.070 ± 0.008	0.069 ± 0.008
		MARD	1.769 ± 0.232	1.628 ± 0.213	1.624 ± 0.213	1.557 ± 0.204	1.537 ± 0.202

Table XIV. Deviations for bulk modulus of 44 cubic solids.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	12.238 ± 1.70	10.277 ± 1.50	10.494 ± 1.52	10.951 ± 1.57	11.264 ± 1.60
		MD	-11.110 ± 1.87	-8.691 ± 1.71	-9.035 ± 1.73	-9.641 ± 1.76	-10.026 ± 1.78
		MARD	11.051 ± 1.71	9.168 ± 1.50	9.230 ± 1.54	9.636 ± 1.58	9.831 ± 1.61
*lp*lsRPBE	PBE	MAD	17.863 ± 2.31	14.697 ± 1.95	15.135 ± 2.01	15.947 ± 2.08	16.481 ± 2.14
		MD	-17.444 ± 2.39	-14.202 ± 2.03	-14.670 ± 2.09	-15.524 ± 2.15	-16.089 ± 2.21
		MARD	15.892 ± 2.33	13.352 ± 1.96	13.516 ± 2.02	14.178 ± 2.10	14.510 ± 2.16
*lp*CAP	PBE	MAD	9.939 ± 1.36	9.015 ± 1.26	9.012 ± 1.26	9.234 ± 1.27	9.319 ± 1.29
		MD	-7.072 ± 1.73	-3.776 ± 1.78	-4.273 ± 1.75	-5.081 ± 1.73	-5.575 ± 1.72
		MARD	12.303 ± 1.41	9.890 ± 1.27	9.820 ± 1.26	10.413 ± 1.28	10.593 ± 1.30
*lp*NCAP	P86	MAD	18.028 ± 2.27	16.790 ± 2.17	16.664 ± 2.15	16.288 ± 2.13	16.079 ± 2.11
		MD	-17.543 ± 2.36	-16.279 ± 2.26	-16.139 ± 2.24	-15.740 ± 2.23	-15.509 ± 2.21
		MARD	16.328 ± 2.29	14.986 ± 2.19	14.992 ± 2.17	14.419 ± 2.15	14.212 ± 2.13

Table XV. Deviations for cohesive energies of 54 solids bounded by strong interactions.

X	C		μ_{MB}	$\mu_{rev}(r_s)$	$\mu_{mod}(r_s)$	$\mu_{HL}(r_s)$	$\mu_{RG}(r_s)$
*lp*PBE	PBE	MAD	0.220 ± 0.03	0.214 ± 0.03	0.244 ± 0.05	0.211 ± 0.03	0.208 ± 0.03
		MD	-0.068 ± 0.04	0.058 ± 0.04	0.084 ± 0.06	0.021 ± 0.04	0.010 ± 0.04
		MARD	5.608 ± 0.74	5.026 ± 0.66	5.707 ± 0.75	5.057 ± 0.67	4.976 ± 0.66
*lp*lsRPBE	PBE	MAD	0.420 ± 0.04	0.291 ± 0.03	0.296 ± 0.03	0.340 ± 0.04	0.337 ± 0.03
		MD	-0.341 ± 0.05	-0.210 ± 0.04	-0.220 ± 0.04	-0.244 ± 0.05	-0.280 ± 0.04
		MARD	9.963 ± 1.31	7.088 ± 0.93	7.130 ± 0.94	8.129 ± 1.07	7.962 ± 1.05
*lp*CAP	PBE	MAD	0.354 ± 0.04	0.297 ± 0.04	0.313 ± 0.05	0.303 ± 0.04	0.308 ± 0.05
		MD	-0.201 ± 0.06	0.083 ± 0.05	0.102 ± 0.06	0.035 ± 0.06	0.043 ± 0.07
		MARD	10.375 ± 1.38	7.502 ± 0.99	7.782 ± 1.03	7.883 ± 1.04	7.928 ± 1.05
*lp*NCAP	P86	MAD	0.513 ± 0.04	0.399 ± 0.03	0.457 ± 0.04	0.380 ± 0.03	0.392 ± 0.03
		MD	-0.484 ± 0.04	-0.351 ± 0.04	-0.315 ± 0.06	-0.327 ± 0.04	-0.342 ± 0.04
		MARD	13.939 ± 1.84	10.736 ± 1.42	12.143 ± 1.61	10.248 ± 1.36	10.748 ± 1.42