Supplemental Information
Reworking the *Tao–Mo* exchange-correlation functional: II. De-orbitalization

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We provide tabulation of the results for use of PBE correlation with *v2-sreg*TM-L, graphical comparisons of exchange enhancment factors for original and de-orbitalized versions of *rreg*TM in the C_2H_2 and C_3H_4 molecules, atomic exchange potentials for two different de-orbitalizations, plots of the functional derivative of the X energy density with respect to the KS kinetic energy density ($\delta e_x/\delta\tau_s$), plots of two cases in which the earlier regularization $z' < 0$, detailed results on $3d$ elememtal magnetiztion, and comparative information on the number of SCF steps. We also provide detailed, system-by-system tabulation of the numerical results for testing against standard molecular and crystalline system data sets.

LIST OF TABLES

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I. DE-ORBITALIZATION RESULTS FOR *v2-sreg*TM-L X PLUS PBE C

Tables I and II present the results obtained from the combination of our deorbitalized X functional *v2-sreg*TM-L (PC_{rep}) with PBE C [1]. These results are compared with the parent functional combination *v2-sreg*TM X + PBE C. Additionally, a comparison is made with the primary outcomes of *v2-sreg*TM-L (PC_{rep}) and *v2-sreg*TM, as illustrated. System-by-system results are tabulated in Sections VII and VIII below.

TABLE I. Summary of molecular test set results for the *v2-sreg*TM-L exchange functional (with $\epsilon_p = 0.5$ and PC_{rep}) combined with the *rreg*TM-L correlation functional and also with PBE C, versus *v2-sreg*TM X combined with PBE C, all compared with *v2-sreg*TM and *rreg*TM. Heat of formation errors in $kcal/mol$, bond length errors in $\mathring{A}$, and frequency errors in cm^{-1}.

	X C	*rreg*TM *rreg*TM	*v2-sreg*TM *rreg*TM	*v2-sreg*TM-L *rreg*TM-L	*v2-sreg*TM *PBE*	*v2-sreg*TM-L *PBE*
Heats of Formation		-3.790	-3.512	8.675	-1.520	9.221
		5.612	5.895	11.471	5.354	15.062
Bonds		0.012	0.013	0.014	0.008	0.010
		0.014	0.015	0.017	0.011	0.016
Frequencies		-21.011	-19.275	-32.277	-2.865	-19.712
		35.578	34.272	43.491	24.138	36.220

TABLE II. Comparison of solid system errors for DFA combinations as in Table I for four solid test sets. Equilibrium lattice constant errors in $\mathring{A}$, cohesive energy errors in $eV/atom$, bulk modulus errors in GPa, and Kohn-Sham band gap errors in eV.

	X C	*rreg*TM *rreg*TM	*v2-sreg*TM *rreg*TM	*v2-sreg*TM-L *rreg*TM-L	*v2-sreg*TM *PBE*	*v2-sreg*TM-L *PBE*
Lattice constants		0.000	0.004	0.018	-0.002	0.012
		0.029	0.031	0.041	0.029	0.035
Cohesive energies		0.212	0.159	0.010	0.199	0.140
		0.251	0.216	0.205	0.251	0.260
Bulk moduli		1.856	0.223	-3.265	2.732	-0.027
		6.740	6.602	8.747	6.542	9.249
Band Gaps		-1.52	-1.53	-1.73	-1.44	-1.73
		1.52	1.53	1.73	1.44	1.73

II. EXCHANGE ENHANCEMENT FACTORS

Figures 1 and 2 display the X enhancement factor behavior of the *rreg*TM functionals and their corresponding deorbitalized versions for C_2H_2 and C_3H_4.

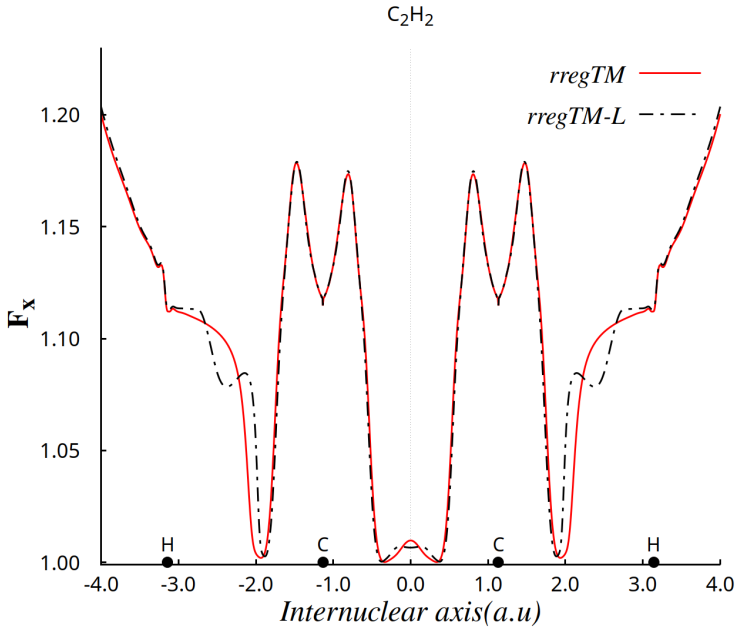

FIG. 1. Enhancement factor F_X for *rreg*TM and *rreg*TM-L (PC_{new}) functionals for C_2H_2 molecule.

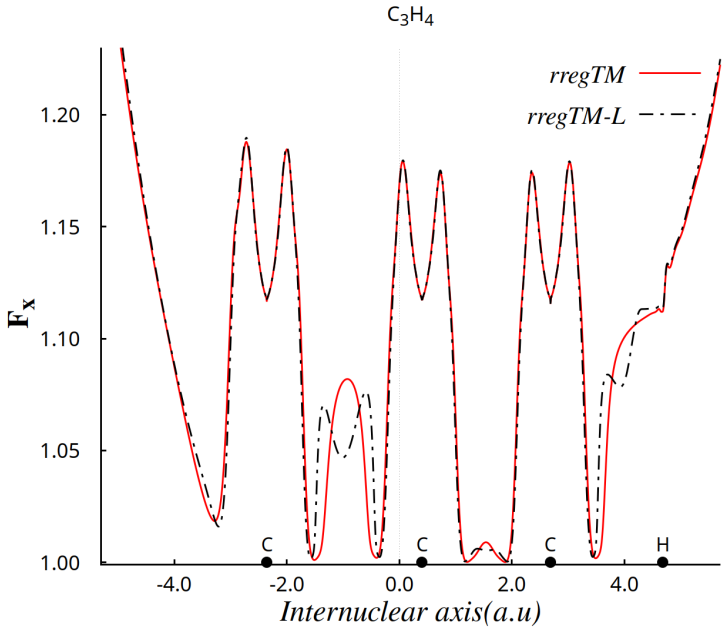

FIG. 2. As in Fig. 1, but for C_3H_4 molecule.

III. EXCHANGE POTENTIAL FOR DEORBITALIZED FUNCTIONALS

Figs. 3 and 4 compare the behavior of the exchange potential for two atoms from the two primary deorbitalized exchange functionals, specifically *v2-sreg*TM-L and *rreg*TM-L. These potential profiles were obtained using a modified version of the Python code `densities` [2]. The code uses analytic Hartree-Fock densities (spherical). The plots utilize 10000 radial points. Note that these potentials are not multiplied by r^2.

From the graphical representations, it is evident that the X potential in deorbitalized functionals exhibits non-smooth behavior, characterized by oscillations near zero. Note that *v2-sreg*TM-L produces slightly less noise than *rreg*TM-L in both systems.

Figs. 5 through 8 compare the exchange potential from a parent meta-GGA (*rreg*TM and *v2sreg*-TM) with its de-orbitalized form. For the parent functional, what is plotted is the *local* part of the non-local gKS potential.

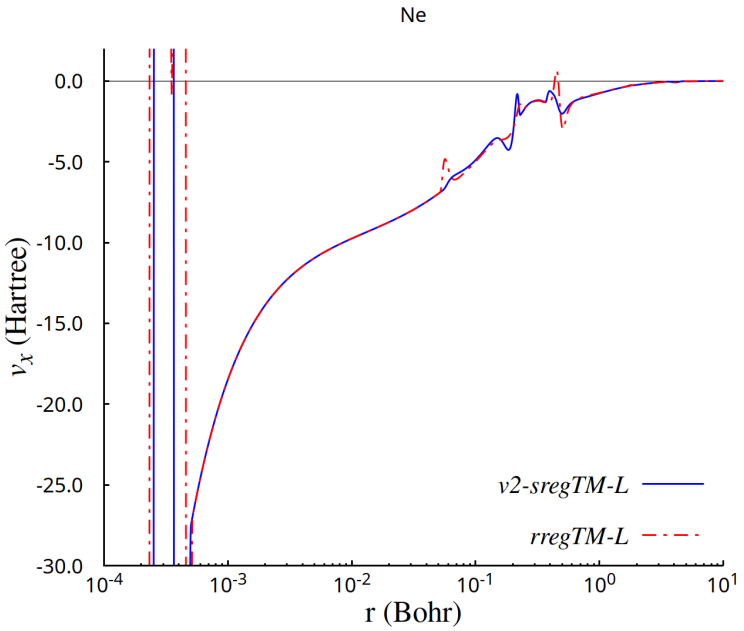

FIG. 3. Exchange potential for the Ne atom, employing the *v2-sreg*TM-L (PC_{rep}) and *rreg*TM-L (PC_{new}) X functionals.

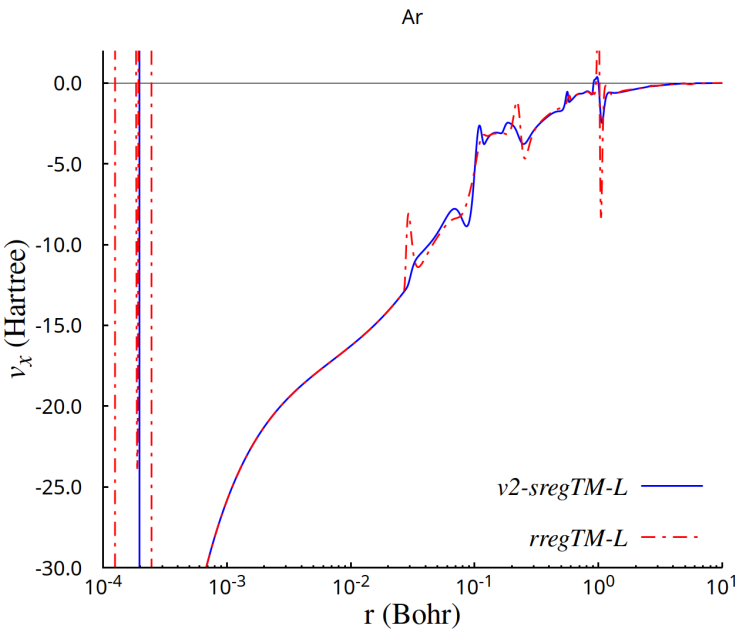

FIG. 4. As in Fig. 3, but for the Ar atom.

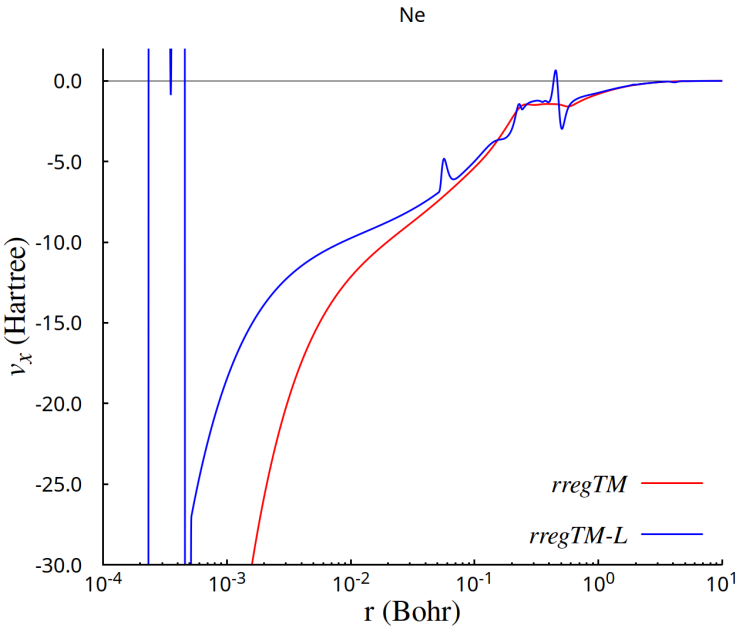

FIG. 5. Exchange potential for the Ne atom, employing the *rreg*TM and *rreg*TM-L (PC_{new}) X functionals. For the parent meta-GGA only the local part of the potential is plotted.

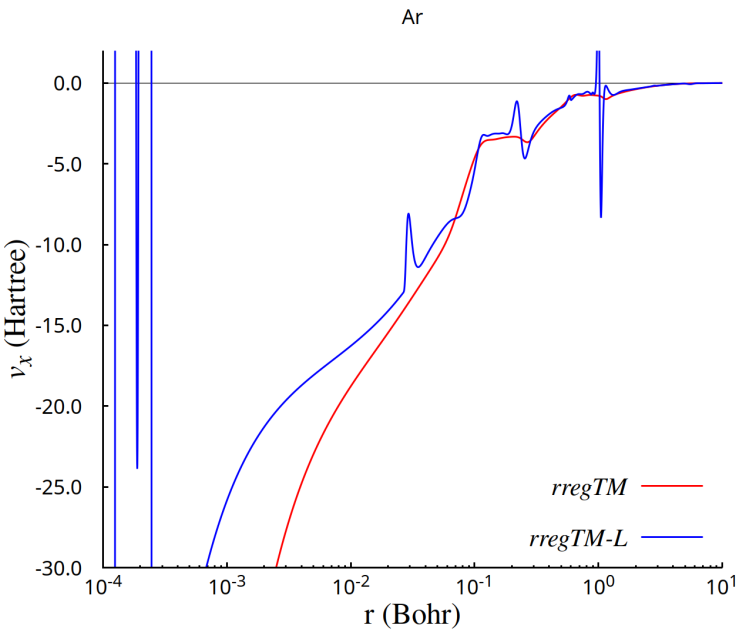

FIG. 6. As in Fig. 5, but for the Ar atom.

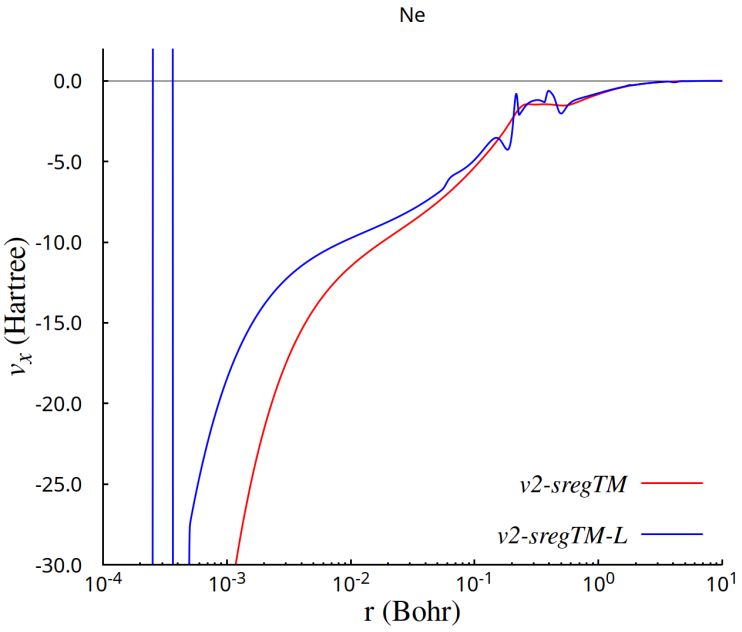

FIG. 7. X potential for the Ne atom, employing the *v2-sreg*TM and *v2-sreg*TM-L (PC_{rep}) exchange functionals. For the parent meta-GGA only the local part of the potential is plotted.

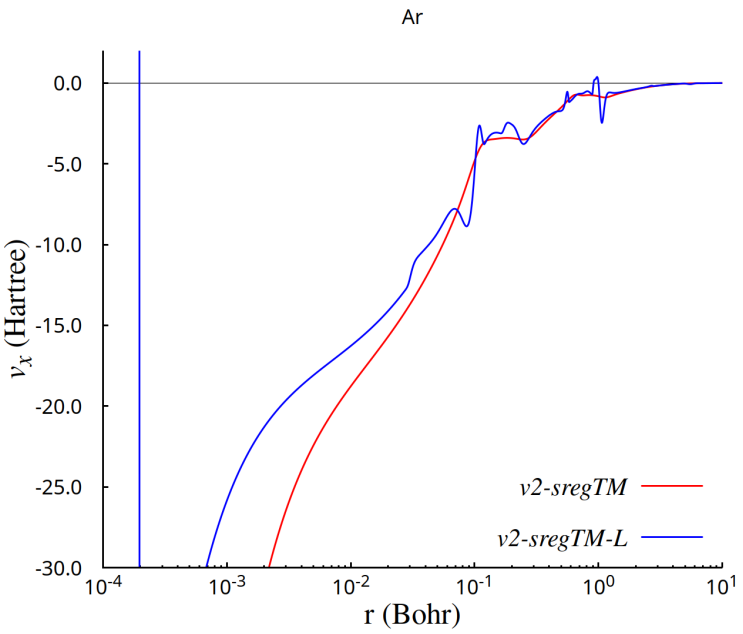

FIG. 8. As in Fig. 7, but for the Ar atom.

Figures 9, 10, and 11 display the derivative of the exchange energy density (e_x) with respect to the KS kinetic energy density (τ_s) for three specific systems: the Ne and Ar atoms, and the C_3H_4 molecule. Figs. 12, 13, and 14 show this derivative but now as a function of the radial coordinate for the atoms and the axial coordinate for C_3H_4. Figs. 15, 16, and 17 show it plotted against α. This derivative is expressed as

$$\frac{\partial e_x(n, \nabla n, \tau_s)}{\partial \tau_s} = A_x n(\mathbf{r})^{4/3} \frac{\partial F_x}{\partial \tau_s} \, . \tag{1}$$

Here, A_x is defined as

$$A_x = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} \, , \tag{2}$$

$n(\mathbf{r})$ is the electronic density, ∇n its gradient, and F_x corresponds to the exchange enhancenment factor, specifically *v2-sreg*TM or *rreg*TM in our particular case.

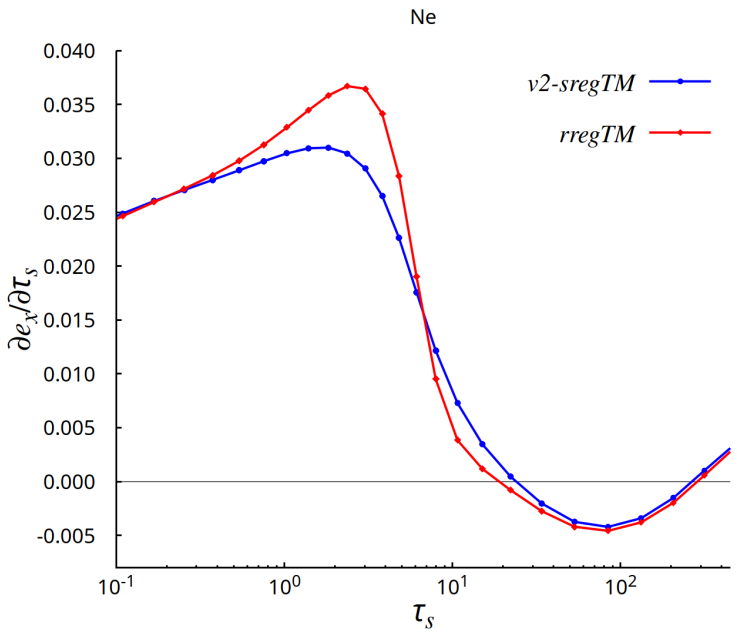

FIG. 9. Derivative of the echange energy density e_x with respect to the kinetic energy density τ_s for the Ne atom, employing the *rreg*TM and *v2-sreg*TM X functionals.

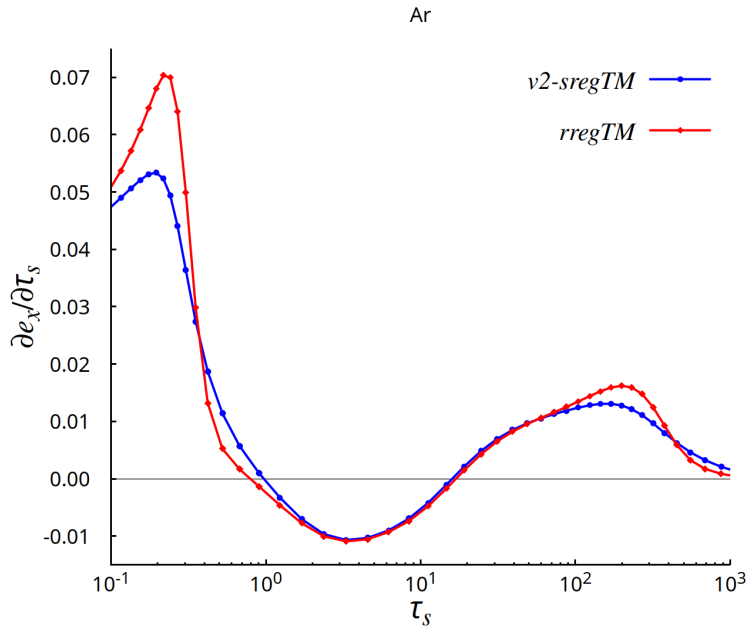

FIG. 10. As in Fig. 9, but for the Ar atom.

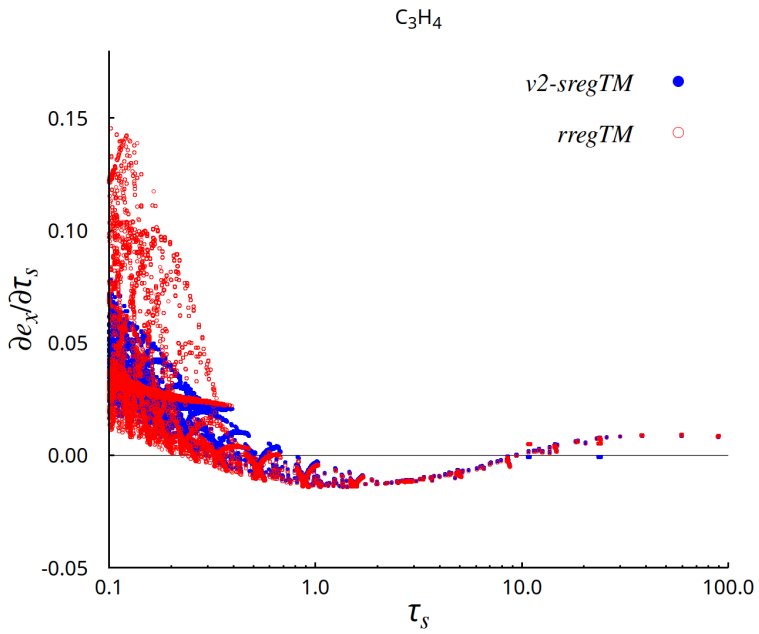

FIG. 11. As in Fig. 9, but for the C_3H_4 molecule.

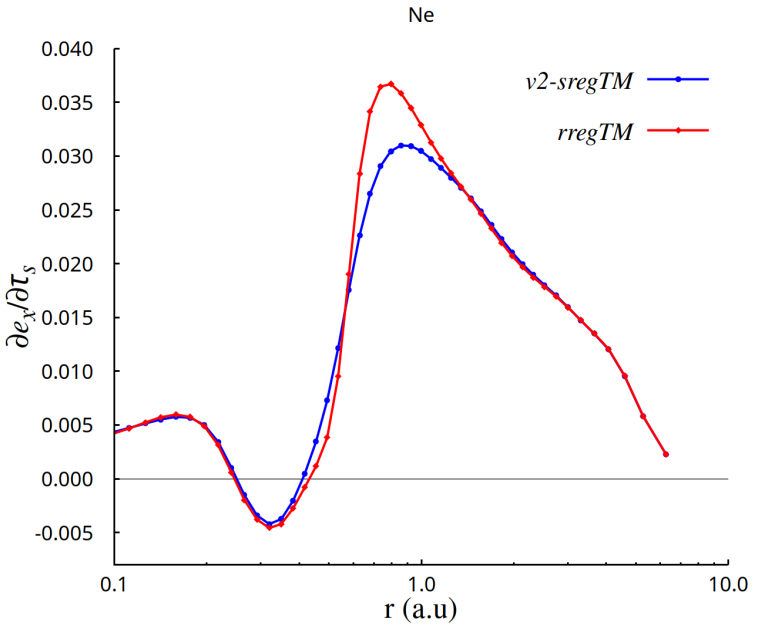

FIG. 12. Derivative of the echange energy density e_x with respect to the kinetic energy density τ_s as a function of the radial coordinate r for the Ne atom, employing the *rreg*TM and *v2-sreg*TM X functionals.

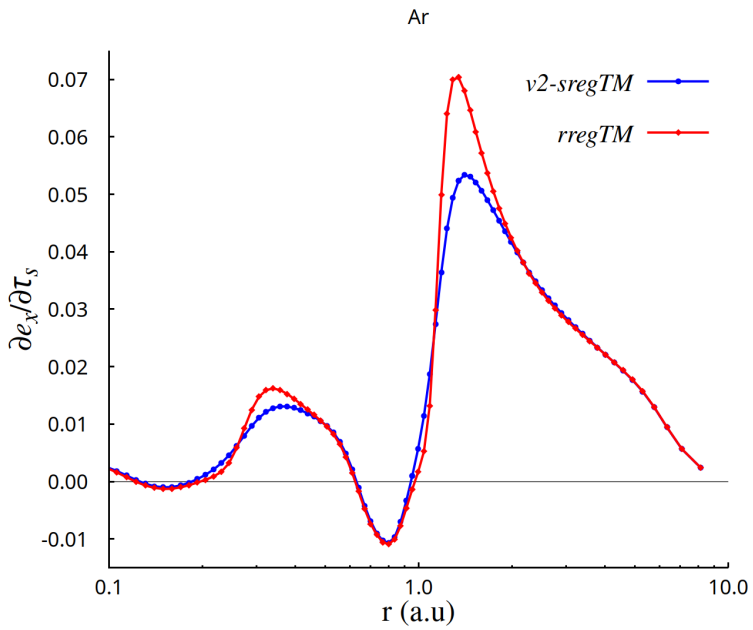

FIG. 13. As in Fig. 12, but for the Ar atom.

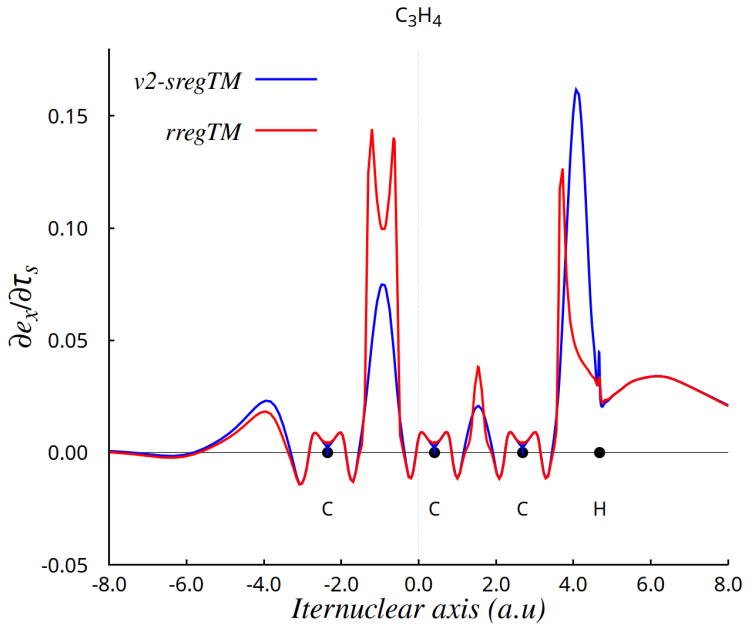

FIG. 14. As in Fig. 12, but for the C_3H_4 molecule. In this case, the plot is along the internuclear axis.

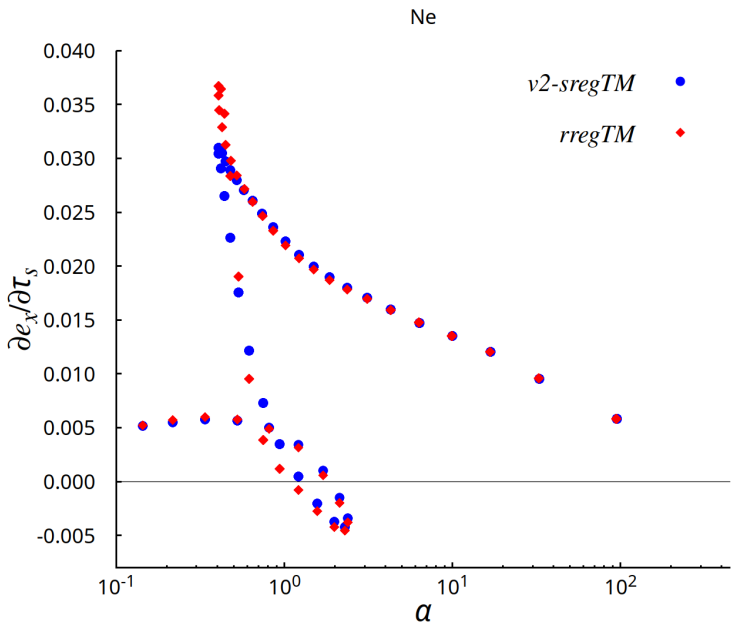

FIG. 15. Derivative of the echange energy density e_x with respect to the KS KE density τ_s plotted as a function of α for the Ne atom, employing the *rreg*TM and *v2-sreg*TM X functionals.

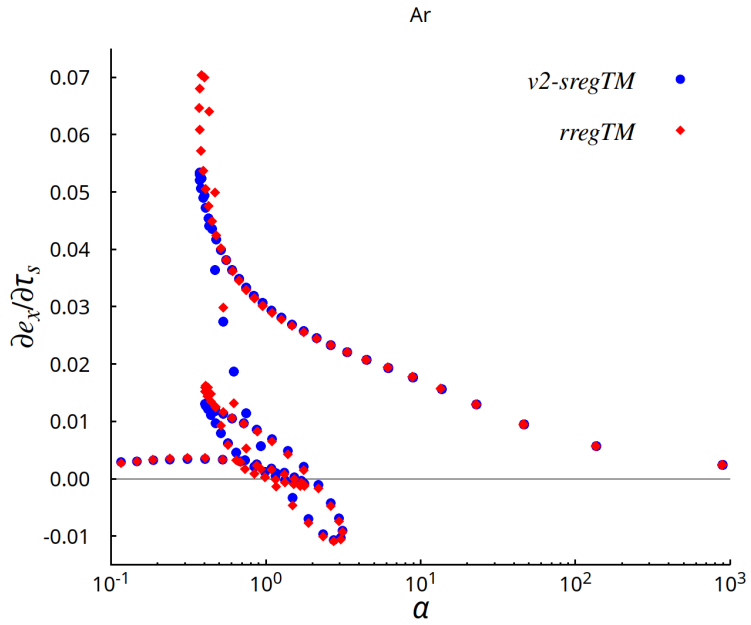

FIG. 16. As in Fig. 15, but for the Ar atom.

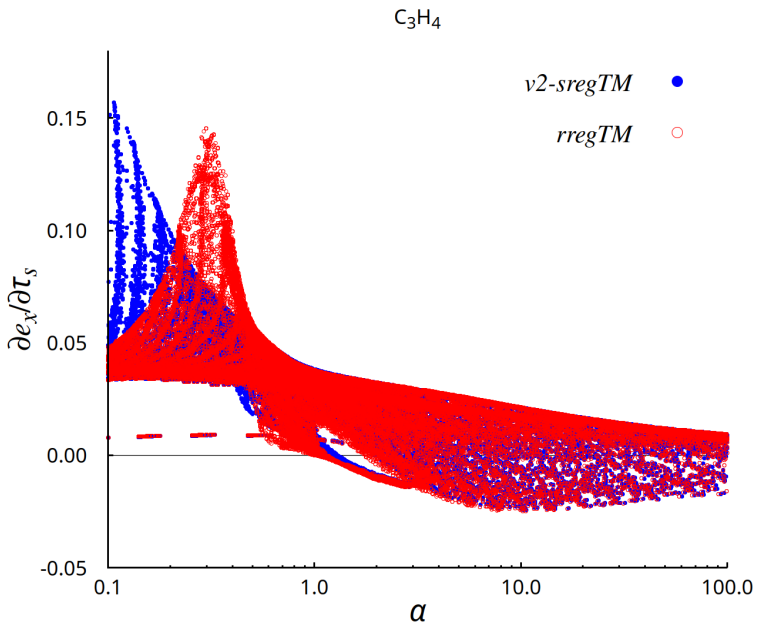

FIG. 17. As in Fig. 15, but for the C_3H_4 molecule.

IV. INDICATOR FUNCTION PLOTS

Figs. 18 and 19 provide two examples of cases for which $z' < 0$, namely in the C_2 and BeH molecules. Both show negative, small magnitude z' in the binding region.

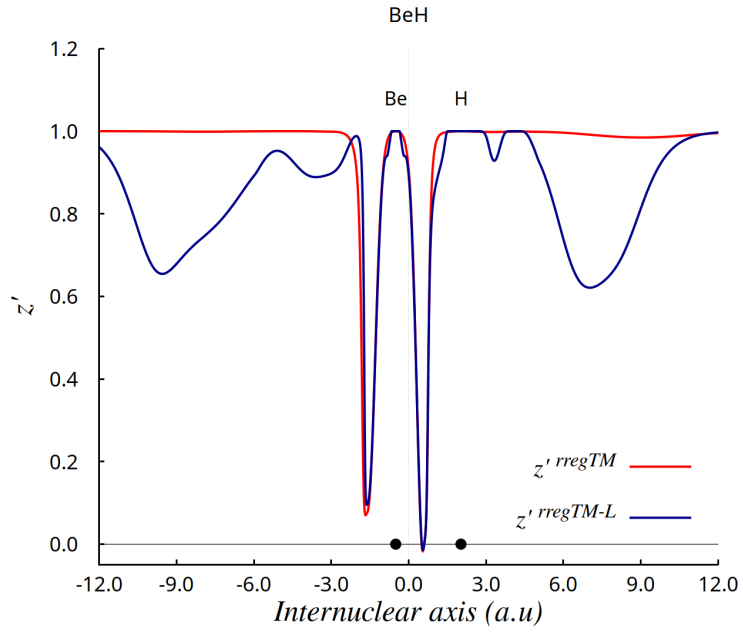

FIG. 18. Orbital-dependent z' and its de-orbitalized approximation using PC_{new} for BeH molecule

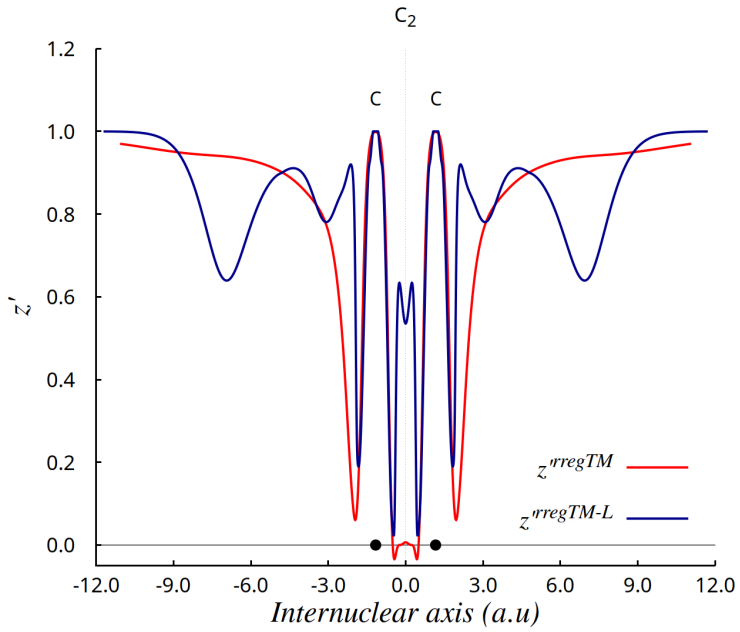

FIG. 19. As in Fig. 18, but for C_2 molecule.

V. MAGNETIZATION ENERGETICS

Here we present information on the magnetization of fcc Fe, fcc Co, fcc Ni, and hcp Co and their fixed spin-moment energy.

TABLE III. Energy of bcc Fe and its saturation magnetic moments for the different functionals sorted in descending order. "Exp." denotes the experimental saturation magnetization.

XC functional	Energy eV	Magnetization μ_B
Exp.		2.22
PBE	-0.5293	2.18
*rreg*TM	-0.6535	2.10
*v2-sreg*TM	-0.6751	2.17
*v2-sreg*TM-L (PC_{rep})	-0.6880	2.15

TABLE IV. As in Table III for fcc Co.

XC functional	Energy eV	Magnetization μ_B
Exp.		1.72
PBE	-0.2055	1.64
*v2-sreg*TM	-0.2946	1.73
*rreg*TM	-0.2996	1.72
*v2-sreg*TM-L(PC_{rep})	-0.3045	1.75

TABLE V. As in Table III for fcc Ni.

XC functional	Energy eV	Magnetization μ_B
Exp.		0.62
PBE	-0.0583	0.63
*v2-sreg*TM	-0.0814	0.66
*v2-sreg*TM-L(PC$_{rep}$)	-0.0856	0.69
*rreg*TM	-0.0875	0.68

TABLE VI. As in Table III for hcp Co.

XC functional	Energy eV	Magnetization μ_B
Exp.		1.57
PBE	-0.2369	1.60
*v2-sreg*TM	-0.2808	1.61
*rreg*TM	-0.2934	1.63
*v2-sreg*TM-L(PC$_{rep}$)	-0.3107	1.65

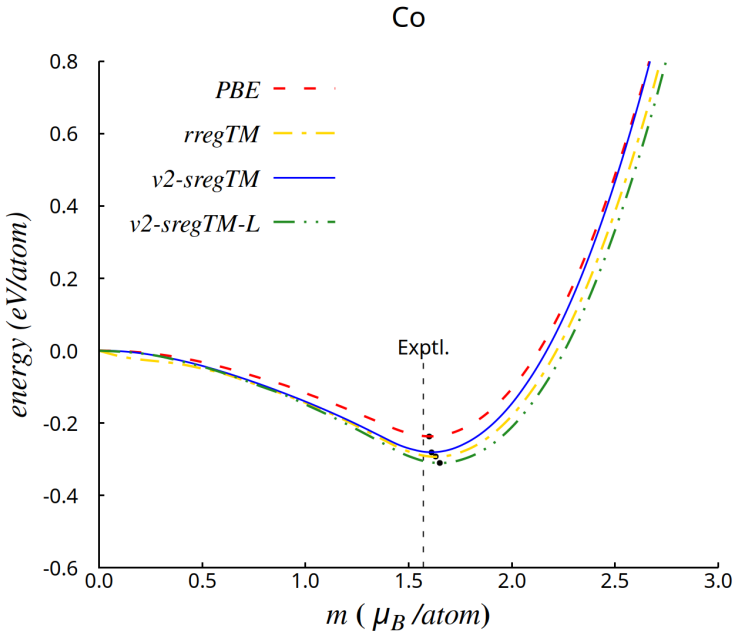

FIG. 20. Fixed spin moment energy for hcp Co using calculated equilibrium latticce parameter, on a per-atom basis for. Comparation of different functionals.

VI. SCF STEPS

Here we show the number of iteratives steps for the molecular test sets. The total number of steps refers to the sum of all SCF steps of each molecule.

TABLE VII. Total number of SCF steps for the molecular test sets.

	*rreg*TM	*rreg*TM-L(PC_{new})	*v2-sreg*TM	*v2-sreg*TM-L (PC_{rep})
Heats of Formation	1774	1984	1764	1960
Bond distances	1851	2297	1848	2121
Frequencies	1967	2427	1951	3028

TABLE VIII. Average of the total number of SCF steps for the molecular test sets.

	*rreg*TM	*rreg*TM-L(PC_{new})	*v2-sreg*TM	*v2-sreg*TM-L (PC_{rep})
Heats of Formation	7.96	8.90	7.91	8.79
Bond distances	19.28	23.93	19.25	22.09
Frequencies	23.98	29.60	23.79	36.93

VII. MOLECULAR TEST SET RESULTS

Here we provide the molecule-by-molecule tabulation for the G3/99, T96R, and T82-F test sets for *v2-sreg*TM compared with its deorbitalized version *v2-sreg*TM-L (PC_{rep}). Also provided are results for *v2-sreg*TM X plus PBE C and its deorbitalized version *v2-sreg*TM-L X (PC_{rep}) plus PBE C.

TABLE IX: Standard enthalpies of formation (ΔH_f) in kcal/mol for the G3X/99 molecular test set [3, 4] obtained with different approximate exchange-correlation functionals.

Molecule	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
LiH	33.30	35.926	37.284	38.815	38.169
^{2}BeH	81.70	77.000	74.768	74.531	76.508
^{2}CH	142.50	141.954	142.202	140.695	143.747
CH_2 ($^3B_1$)	93.60	90.538	90.224	91.891	97.215
CH_2 ($^1A_1$)	102.60	107.274	108.592	105.401	110.748
$^3CH_3$	35.00	34.291	34.283	34.936	43.437
CH_4	-17.80	-14.357	-9.709	-13.697	-2.208
^{3}NH	85.80	78.907	77.096	79.532	82.165
NH_2 ($^2B_1$)	44.50	38.827	35.920	40.560	44.681
NH_3	-10.90	-10.516	-9.379	-7.192	-2.260
^{2}OH	9.00	8.412	5.901	11.021	11.118
H_2O	-57.80	-51.885	-50.486	-46.389	-46.685
HF	-65.20	-59.707	-55.257	-55.930	-57.251
SiH_2 ($^1A_1$)	65.20	67.616	69.870	64.883	70.027
SiH_2 ($^3B_1$)	86.20	82.261	81.795	81.012	87.257
$^2SiH_3$	47.90	46.795	48.154	43.465	53.648
SiH_4	8.20	11.422	15.326	6.161	20.610
$^2PH_2$	33.10	29.389	31.084	27.951	33.747
PH_3	1.30	2.198	6.267	-0.249	8.574
H_2S	-4.90	-3.314	-0.167	-2.315	1.119
HCl	-22.00	-20.189	-17.948	-18.496	-16.843
Li_2	51.60	55.253	56.816	57.626	57.003
LiF	-80.10	-73.943	-68.852	-70.754	-72.996
HC≡CH	54.60	54.842	59.021	56.714	58.625
$H_2C{=}CH_2$	12.50	14.063	20.647	14.350	25.741
$H_3C{-}CH_3$	-20.10	-15.872	-7.203	-15.200	2.759
CN	105.20	95.991	95.698	98.190	92.201
HCN	30.90	26.513	28.515	27.082	25.704
CO	-26.40	-26.197	-21.458	-24.768	-29.004
^{2}HCO	10.00	3.544	5.826	6.123	4.663
H_2CO	-26.10	-26.585	-22.830	-25.910	-22.843
CH_3OH	-48.00	-44.273	-38.885	-41.343	-32.815
N_2	0.00	-8.310	-7.407	-9.381	-13.193
H_2NNH_2	23.30	21.633	22.556	24.896	31.484
NO	21.80	10.969	10.055	11.676	7.302
$^3O_2$	0.00	-11.978	-14.199	-9.316	-15.668
H_2O_2	-32.40	-33.107	-34.165	-27.951	-31.107
F_2	0.00	-5.876	-3.418	-5.948	-10.480
CO_2	-94.00	-101.750	-95.284	-97.391	-104.433
Na_2	34.00	33.547	34.101	36.162	36.507
Si_2	139.90	137.319	136.161	139.427	133.271
P_2	34.30	31.588	37.390	31.340	27.111

(continued)

$^3S_2$	30.70	21.211	24.789	23.224	19.116
Cl_2	0.00	-1.991	0.804	-1.919	-4.065
NaCl	-43.60	-39.969	-37.856	-38.386	-36.991
SiO	-24.60	-21.404	-18.407	-19.597	-23.721
CS	66.90	65.091	69.974	66.335	61.489
SO	1.20	-6.696	-5.284	-4.428	-9.381
ClO	24.30	15.690	15.144	16.666	13.216
ClF	-13.30	-15.961	-11.674	-15.989	-18.679
Si_2H_6	19.10	22.010	28.978	13.019	37.185
CH_3Cl	-19.60	-18.498	-13.041	-18.311	-9.498
H_3C-SH	-5.50	-3.774	2.906	-3.086	7.123
HOCl	-18.40	-19.445	-18.244	-16.816	-19.450
SO_2	-71.00	-74.613	-68.310	-71.332	-77.658
BF_3	-271.40	-266.884	-247.701	-261.526	-263.594
BCl_3	-96.30	-101.186	-92.776	-97.696	-98.642
AlF_3	-289.00	-278.277	-261.104	-274.062	-275.366
$AlCl_3$	-139.70	-141.054	-132.586	-138.614	-136.161
CF_4	-223.10	-227.853	-202.005	-222.543	-225.439
CCl_4	-22.90	-30.434	-20.526	-27.643	-32.178
OCS	-33.10	-44.541	-37.378	-40.958	-47.564
CS_2	28.00	14.598	22.809	17.758	11.757
F_2CO	-145.00	-151.854	-135.959	-147.085	-152.247
SiF_4	-386.00	-372.539	-344.942	-367.703	-366.364
$SiCl_4$	-158.40	-159.900	-145.873	-157.307	-154.094
NNO	19.70	-3.102	-1.617	-1.311	-9.505
ClNO	12.60	-6.901	-7.043	-5.256	-13.895
NF_3	-31.60	-53.044	-44.243	-51.654	-58.592
PF_3	-229.10	-226.830	-206.283	-224.894	-225.298
O_3	33.90	18.573	14.746	21.096	9.199
F_2O	5.90	-9.364	-7.919	-8.912	-16.737
ClF_3	-38.00	-56.919	-46.357	-54.115	-62.419
$F_2C=CF_2$	-161.30	-172.793	-145.704	-167.401	-171.845
$Cl_2C=CCl_2$	-5.50	-16.672	-2.276	-12.968	-16.309
F_3C-CN	-118.40	-131.919	-110.257	-127.682	-133.362
$HC\equiv C-CH_3$	44.40	43.923	53.220	46.624	55.351
$H_2C=C=CH_2$	45.40	40.997	50.505	43.372	52.808
C_3H_4 (cyclopropene)	67.80	63.498	73.104	65.508	74.525
$H_2C=CH-CH_3$	4.80	6.483	17.663	7.432	25.146
C_3H_6 (cyclopropane)	12.80	12.159	24.517	13.638	31.322
$CH_3-CH_2-CH_3$	-25.10	-20.048	-7.222	-19.191	5.156
C_4H_6 (Z-1,3-butadiene)	26.40	24.901	38.523	25.744	43.530
C_4H_6 (2-butyne)	34.80	34.699	49.037	38.067	53.622
C_4H_6 (methylenecyclopropane)	47.90	41.325	56.662	43.782	60.813
C_4H_6 (bicyclo[1.1.0]butane)	51.90	47.171	62.953	49.685	66.107
C_4H_6 (cyclobutene)	38.20	36.265	50.908	37.117	55.503
C_4H_8 (cyclobutane)	6.60	7.924	24.140	8.349	33.878
C_4H_8 (isobutene)	-4.10	-1.784	13.897	-0.281	23.696
C_4H_{10} (trans butane)	-30.10	-24.188	-7.166	-23.148	7.585
C_4H_{10} (isobutane)	-32.20	-26.139	-9.121	-25.019	5.579
C_5H_8 (spiropentane)	44.30	38.575	59.510	41.479	65.393
C_6H_6 (benzene)	19.90	10.751	33.248	12.330	32.670
CH_2F_2	-107.70	-108.092	-94.508	-107.109	-101.617

(continued)

CHF_3	-166.30	-169.145	-149.574	-166.249	-164.785
CH_2Cl_2	-22.60	-24.119	-17.268	-23.521	-18.567
$CHCl_3$	-24.50	-28.816	-20.381	-27.233	-26.771
CH_3NH_2	-5.20	3.078	7.964	4.643	17.733
CH_3CN	18.00	12.359	19.553	13.763	19.469
CH_3NO_2 (nitromethane)	-17.90	-35.135	-29.418	-32.960	-30.640
CH_3ONO (methyl nitrite)	-16.10	-32.778	-28.319	-31.293	-29.345
CH_3SiH_3	-7.00	-1.883	6.345	-5.122	15.627
HCO_2H	-90.40	-93.062	-86.138	-88.011	-88.344
HCO_2CH_3	-85.50	-89.807	-78.940	-87.341	-78.772
CH_3CONH_2	-57.00	-62.664	-51.249	-57.904	-47.222
C_2H_5N (aziridine)	30.20	23.947	32.642	25.197	38.567
NCCN (cyanogen)	74.10	56.628	61.566	58.096	50.654
$NH(CH_3)_2$	-4.30	-4.316	5.133	-3.513	16.524
$CH_3CH_2NH_2$	-11.30	-11.398	-1.923	-9.052	9.858
$H_2C{=}C{=}O$ (ketene)	-11.60	-19.314	-11.429	-15.299	-14.693
C_2H_4O (oxirane)	-12.60	-16.563	-7.953	-15.658	-5.146
CH_3CHO	-39.50	-40.420	-31.628	-38.611	-29.146
$O{=}CH{-}CH{=}O$	-50.80	-56.157	-48.080	-54.157	-52.958
CH_3CH_2OH	-56.10	-51.927	-42.155	-48.616	-33.653
$(CH_3)_2O$	-44.00	-41.997	-32.372	-41.531	-24.257
C_2H_4S (thiooxirane)	19.60	15.142	25.131	15.899	26.259
$(CH_3)_2S{=}O$	-36.20	-36.976	-23.898	-34.504	-19.186
CH_3CH_2SH	-11.10	-8.389	2.455	-7.478	8.939
$(CH_3)_2S$	-8.90	-7.328	3.173	-6.644	10.156
$H_2C{=}CHF$	-34.00	-35.950	-24.452	-34.467	-26.867
CH_3CH_2Cl	-26.60	-25.114	-15.404	-24.574	-8.600
$H_2C{=}CHCl$	5.20	3.183	11.493	4.300	12.770
$H_2C{=}CHCN$	43.20	36.280	45.639	37.435	43.047
$(CH_3)_2C{=}O$	-51.70	-52.295	-38.728	-49.578	-33.660
CH_3CO_2H	-103.40	-105.301	-93.553	-99.338	-93.134
CH_3CFO	-105.70	-109.179	-94.597	-105.555	-99.829
CH_3COCl	-57.70	-63.993	-53.592	-60.610	-54.859
$CH_3CH_2CH_2Cl$	-31.50	-29.214	-15.339	-28.506	-6.592
$(CH_3)_2CHOH$	-65.20	-60.636	-46.491	-56.820	-35.585
$CH_3{-}O{-}CH_2CH_3$	-51.70	-49.498	-35.467	-48.641	-24.895
$(CH_3)_3N$	-6.60	-6.558	7.207	-6.923	20.492
C_4H_4O (furan)	-8.30	-17.894	-1.445	-15.022	-4.544
C_4H_4S (thiophene)	27.50	18.184	35.827	20.730	31.296
C_4H_5N (pyrrole)	25.90	13.806	30.608	16.834	30.967
C_5H_5N (pyridine)	33.60	18.374	38.006	19.005	35.594
H_2	0.00	1.322	3.357	3.877	7.735
^2SH	34.20	33.094	33.924	33.713	35.302
$^2C{\equiv}CH$	135.80	132.258	133.836	135.206	133.532
$HC{=}CH_2$ ($^2A'$)	71.00	66.638	70.010	68.485	75.864
$CH_3C{=}O$ ($^2A'$)	-2.40	-8.999	-2.326	-5.808	-0.416
$CH_2{-}OH$ (^2A)	-4.00	-5.957	-3.625	-2.017	2.911
CH_3O ($^2A'$)	5.20	-0.441	2.181	0.953	8.789
CH_3CH_2O ($^2A''$)	-2.90	-8.881	-1.784	-6.862	7.188
CH_3S ($^2A'$)	29.80	27.084	31.813	27.874	35.920
CH_2CH_3 ($^2A'$)	28.60	27.898	32.606	29.235	44.083
$(CH_3)_2CH$ ($^2A'$)	21.10	20.243	29.672	22.260	43.439

(continued)

$^2C(CH_3)_3$	12.00	11.922	25.998	14.501	41.945
NO_2 ($^2A_1$)	8.10	-15.256	-15.511	-12.234	-21.034
$CH_3CH{=}C{=}CH_2$	38.80	35.268	49.163	37.954	53.928
C_5H_8 (isoprene)	18.00	17.244	35.291	18.578	42.580
C_5H_{10} (cyclopentane twist)	-18.50	-14.579	6.165	-13.738	18.306
C_5H_{12} (n-pentane)	-35.00	-28.262	-7.064	-27.050	9.967
$C(CH_3)_4$ (neopentane)	-40.10	-33.340	-12.163	-31.976	4.806
C_6H_8 (1,3-cyclohexadiene)	25.40	23.377	45.989	25.105	50.582
C_6H_8 (1,4-cyclohexadiene)	25.00	23.891	46.781	25.863	51.326
C_6H_{12} (cyclohexane chair)	-29.40	-23.923	1.460	-22.844	15.782
C_6H_{14} (n-hexane)	-39.90	-32.355	-7.052	-30.966	12.416
C_6H_{14} (3-methylpentane)	-41.10	-32.852	-7.596	-31.512	11.557
$C_6H_5{-}CH_3$ (toluene)	12.00	3.800	30.787	6.023	32.582
C_7H_{16} (n-heptane)	-44.80	-36.439	-6.892	-34.875	14.973
C_8H_8 (cyclooctatetraene)	70.70	63.800	91.759	66.287	91.573
C_8H_{18} (n-octane)	-49.80	-40.534	-6.810	-38.794	17.434
$C_{10}H_8$ (naphtalene)	35.90	16.698	54.657	19.578	48.295
$C_{10}H_8$ (azulene)	69.10	48.147	84.996	51.337	78.982
$CH_3CO_2CH_3$ (Z-methylacetate)	-98.40	-101.548	-85.829	-98.209	-83.059
$(CH_3)_3COH$ (t-butanol)	-74.70	-69.498	-51.058	-65.227	-37.774
$C_6H_5NH_2$ (aniline)	20.80	6.037	30.370	10.447	31.128
C_6H_5OH (phenol)	-22.30	-33.266	-8.723	-27.717	-11.346
C_4H_6O (divinyl ether)	-3.30	-7.958	7.632	-5.319	10.046
C_4H_8O (tetrahydrofuran)	-44.00	-42.859	-24.826	-42.019	-16.919
C_5H_8O (cyclopentanone)	-45.90	-48.342	-26.482	-45.342	-21.848
$C_6H_4O_2$ (benzoquinone)	-29.40	-43.227	-20.013	-39.911	-29.785
$C_6H_4N_2$ (pyrimidine)	46.80	24.048	41.035	23.810	36.704
$(CH_3)_2SO_2$	-89.20	-89.919	-71.599	-85.520	-69.213
C_6H_5Cl (chlorobenzene)	12.50	-0.051	24.068	2.376	19.359
$NC(CH_2)_2CN$ (succinonitrile)	50.10	37.301	50.948	39.480	45.766
$C_4H_4N_2$ (pyrazine)	46.90	27.817	44.465	27.497	40.188
C_4H_4O (3-butyn-2-one)	15.60	12.512	25.943	16.643	23.092
C_4H_6O (E-crotonaldehyde)	-24.00	-28.889	-13.106	-26.767	-10.726
$C_4H_6O_3$ (acetic anhydride)	-136.80	-146.158	-124.794	-139.608	-127.618
C_4H_6S (2,5-dihydrothiophene)	20.80	17.289	34.563	18.484	36.015
$(CH_3)_2CHCN$	5.60	3.613	18.896	5.187	23.867
C_4H_8O (methyl ethyl ketone)	-57.10	-56.875	-39.058	-53.944	-31.580
$(CH_3)_2CHCHO$	-51.60	-49.434	-32.404	-47.331	-25.108
$C_4H_8O_2$ (1,4-dioxane)	-75.50	-77.480	-57.961	-76.407	-51.755
C_4H_8S (tetrahydrothiophene)	-8.20	-7.109	11.462	-6.394	17.982
$(CH_3)_3CCl$	-43.50	-41.065	-22.932	-39.763	-11.203
C_4H_9Cl (n-butyl chloride)	-37.00	-33.228	-15.229	-32.370	-3.720
C_4H_9N (tetrahydropyrrole)	-0.80	-2.393	15.194	-1.532	26.401
$C_4H_9NO_2$ (2-nitrobutane)	-39.10	-53.657	-35.186	-50.604	-29.084
$(CH_3CH_2)_2O$	-60.30	-56.886	-38.511	-55.651	-25.509
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	-93.10	-92.304	-72.449	-90.591	-61.428
$(CH_3)_3CSH$	-26.20	-22.649	-3.411	-21.083	7.795
$C_4H_{10}S_2$ (diethyl disulfide)	-17.90	-17.002	4.361	-15.554	12.637
$(CH_3)_3CNH_2$	-28.90	-27.045	-9.035	-24.000	7.454
$(CH_3)_4Si$	-55.70	-44.539	-23.193	-41.109	-2.399
C_5H_6S (2-methyl thiophene)	20.00	11.390	33.477	14.483	31.321
C_5H_7N (N-methyl pyrrole)	24.60	12.838	33.967	14.779	36.533

(continued)

$C_5H_{10}O$ (tetrahydropyran)	-53.40	-51.416	-28.907	-50.295	-18.688
$(CH_3CH_2)_2C{=}O$	-61.60	-61.358	-39.321	-58.227	-29.519
$C_5H_{10}O_2$ (isopropyl acetate)	-115.10	-116.873	-92.500	-112.678	-84.858
$C_5H_{10}S$ (tetrahydrothiopyran)	-15.20	-13.089	9.953	-12.055	18.785
$C_5H_{11}N$ (piperidine)	-11.30	-11.196	10.993	-9.852	24.481
$C_5H_{12}O$ (t-butyl methyl ether)	-67.80	-63.713	-41.211	-62.025	-25.922
$C_6H_4F_2$ (1,3-difluorobenzene)	-73.90	-90.254	-57.726	-85.869	-73.262
$C_6H_4F_2$ (1,4-difluorobenzene)	-73.30	-89.478	-57.028	-85.164	-72.786
C_6H_5F (fluorobenzene)	-27.40	-40.088	-12.588	-37.115	-20.630
$C_6H_{14}O$ (diisopropyl ether)	-76.30	-71.295	-44.368	-69.263	-26.645
PF_5	-381.10	-376.790	-342.453	-371.940	-370.807
SF_6	-291.70	-302.412	-266.269	-295.991	-299.838
P_4	14.10	-4.554	9.633	-4.811	-10.383
SO_3	-94.60	-103.157	-93.755	-97.609	-105.023
SCl_2	-4.20	-10.036	-4.498	-9.299	-12.597
$POCl_3$	-133.80	-140.310	-126.806	-137.130	-138.560
PCl_5	-86.10	-100.744	-87.149	-98.031	-99.635
Cl_2O_2S	-84.80	-95.918	-84.415	-90.533	-96.964
PCl_3	-69.00	-76.270	-67.089	-74.824	-76.885
Cl_2S_2	-4.00	-19.103	-11.139	-16.868	-22.793
$SiCl_2$ ($^1A_1$)	-40.30	-42.012	-34.958	-40.401	-40.828
CF_3Cl	-169.70	-176.882	-155.309	-172.236	-175.568
C_2F_6	-320.90	-332.161	-292.529	-325.326	-327.940
$^2CF_3$	-111.80	-121.275	-104.168	-116.788	-119.492
$^2C_6H_5$ (phenyl radical)	80.50	65.060	84.185	68.046	84.385
ME		-3.512	8.675	-1.520	9.221
MAD		5.895	11.471	5.354	15.062

TABLE X: Bond lengths in $\mathring{A}$ for the T96-R molecular test set [5, 6] from different approximate XC functionals.

Molecule	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
H_2	0.741	0.744	0.746	0.743	0.729
Li_2	2.673	2.736	2.718	2.744	2.647
LiH	1.595	1.606	1.602	1.595	1.580
LiF	1.564	1.579	1.574	1.571	1.567
LiCl	2.021	2.029	2.018	2.018	2.002
LiO	1.688	1.703	1.697	1.692	1.688
Be_2	2.440	2.487	2.438	2.428	2.396
BeH	1.343	1.360	1.357	1.351	1.329
BeF	1.361	1.381	1.379	1.378	1.376
BeO	1.331	1.344	1.343	1.340	1.343
BeS	1.742	1.754	1.748	1.749	1.744
B_2	1.590	1.621	1.610	1.617	1.614
BH	1.232	1.245	1.247	1.237	1.225
BF	1.263	1.273	1.276	1.272	1.278
BF_3	1.313	1.321	1.325	1.319	1.323
BCl	1.715	1.728	1.733	1.722	1.730
BCl_3	1.742	1.744	1.745	1.742	1.740
BN	1.281	1.331	1.329	1.326	1.329
BO	1.204	1.213	1.215	1.210	1.214
BS	1.609	1.618	1.615	1.614	1.615
C_2	1.242	1.399	1.397	1.253	1.400
CH	1.120	1.136	1.133	1.127	1.116
CH_4	1.087	1.093	1.091	1.090	1.081
CF	1.272	1.287	1.295	1.285	1.297
CF_4	1.323	1.332	1.340	1.331	1.339
CCl	1.645	1.663	1.670	1.661	1.671
CCl_4	1.767	1.778	1.785	1.775	1.783
CN	1.172	1.173	1.173	1.171	1.177
CO	1.128	1.134	1.137	1.133	1.138
CO^+	1.115	1.120	1.123	1.118	1.124
CO_2	1.160	1.169	1.174	1.168	1.174
CP	1.562	1.562	1.559	1.559	1.565
CS	1.535	1.543	1.544	1.540	1.547
CS_2	1.553	1.559	1.561	1.557	1.561
N_2	1.098	1.101	1.103	1.099	1.105
N_2^+	1.116	1.113	1.114	1.112	1.117
NH	1.036	1.049	1.050	1.043	1.037
NH^+	1.070	1.088	1.086	1.080	1.068
NF	1.317	1.329	1.343	1.328	1.343
NCl	1.611	1.623	1.634	1.622	1.634
NO	1.151	1.157	1.163	1.155	1.164
NO^+	1.063	1.067	1.071	1.065	1.073
NS	1.494	1.504	1.509	1.501	1.512
O_2	1.208	1.218	1.231	1.218	1.231
O_2^+	1.116	1.120	1.129	1.119	1.130
OH	0.970	0.982	0.982	0.979	0.975
OH^+	1.029	1.044	1.043	1.037	1.029
OF	1.358	1.364	1.375	1.365	1.378
F_2	1.412	1.415	1.426	1.415	1.427

(continued)

F_2^+	1.322	1.315	1.329	1.315	1.331
HF	0.917	0.929	0.931	0.927	0.927
HF^+	1.001	1.020	1.020	1.015	1.012
Na_2	3.079	3.079	3.079	3.130	3.077
NaH	1.887	1.892	1.887	1.887	1.874
NaF	1.926	1.931	1.932	1.929	1.930
NaCl	2.361	2.361	2.355	2.358	2.350
NaO	2.052	2.059	2.059	2.056	2.054
MgH	1.730	1.751	1.749	1.736	1.721
MgF	1.750	1.774	1.775	1.771	1.772
MgCl	2.196	2.214	2.210	2.209	2.202
MgO	1.748	1.744	1.746	1.743	1.746
Al_2	2.466	2.470	2.459	2.466	2.461
AlH	1.648	1.666	1.668	1.654	1.639
AlF	1.654	1.674	1.677	1.671	1.673
AlCl	2.130	2.149	2.151	2.143	2.140
AlO	1.618	1.629	1.632	1.628	1.631
AlS	2.029	2.040	2.037	2.035	2.033
Si_2	2.246	2.157	2.151	2.152	2.266
SiH	1.520	1.538	1.537	1.526	1.511
SiH_4	1.480	1.485	1.484	1.481	1.466
SiF	1.601	1.623	1.629	1.620	1.626
SiF_4	1.553	1.572	1.575	1.571	1.574
SiCl	2.058	2.076	2.080	2.072	2.074
$SiCl_4$	2.019	2.028	2.028	2.026	2.025
SiN	1.572	1.575	1.574	1.572	1.578
SiO	1.510	1.524	1.527	1.521	1.527
SiS	1.929	1.942	1.942	1.938	1.942
P_2	1.893	1.897	1.896	1.893	1.899
P_4	2.210	2.198	2.200	2.194	2.202
PH	1.421	1.436	1.436	1.427	1.414
PF	1.589	1.609	1.619	1.607	1.617
PCl	2.015	2.025	2.034	2.023	2.030
PN	1.491	1.496	1.497	1.493	1.500
PO	1.476	1.492	1.497	1.489	1.498
S_2	1.889	1.905	1.908	1.902	1.912
SH	1.341	1.352	1.350	1.346	1.335
SF	1.601	1.618	1.629	1.616	1.631
SF_6	1.561	1.586	1.599	1.584	1.597
SO	1.481	1.501	1.510	1.499	1.512
SO_3	1.420	1.439	1.448	1.437	1.449
Cl_2	1.988	2.009	2.018	2.008	2.019
Cl_2^+	1.891	1.911	1.919	1.910	1.922
HCl	1.275	1.285	1.284	1.281	1.272
HCl^+	1.315	1.329	1.327	1.322	1.307
ClF	1.628	1.651	1.665	1.650	1.666
ClO	1.570	1.589	1.603	1.589	1.605
ME		0.013	0.014	0.008	0.010
MAD		0.015	0.017	0.011	0.016

TABLE XI: Harmonic vibrational frequencies in cm^{-1} for the T82-F molecular test set [5, 6] obtained with different approximate exchange-correlation functionals.

Molecule	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
H_2	4401.20	4387.61	4364.34	4423.28	4559.61
Li_2	351.40	329.64	339.95	338.47	355.03
LiH	1405.70	1383.55	1377.21	1411.80	1422.29
LiF	910.60	892.81	890.74	906.59	903.57
LiCl	643.00	639.72	643.95	650.72	651.58
LiO	814.60	798.89	797.66	813.97	806.26
LiNa	256.80	249.29	252.25	245.86	258.67
Be_2	267.90	323.90	358.51	352.32	361.17
BeH	2060.80	1984.70	1979.67	2040.48	2094.01
BeH^+	2221.70	2149.13	2157.46	2186.90	2253.54
BeF	1247.40	1206.13	1201.65	1213.90	1206.92
BeCl	846.70	812.56	813.64	821.89	820.86
BeO	1487.30	1468.96	1460.28	1479.45	1450.30
BeS	997.90	988.72	993.53	995.86	985.98
B_2	1051.30	1010.37	1028.39	1013.61	1003.63
BH	2366.90	2273.02	2259.23	2346.24	2344.20
BF	1402.10	1373.97	1350.43	1383.48	1338.72
BCl	840.30	816.44	799.97	831.12	796.31
BN	1514.60	1524.17	1531.44	1544.90	1503.67
BO	1885.70	1854.60	1832.33	1868.82	1827.29
BS	1180.20	1170.51	1169.20	1180.60	1158.82
C_2	1854.70	1860.38	1870.12	1860.90	1819.69
CH	2858.50	2726.40	2753.91	2808.77	2826.09
CF	1308.10	1263.46	1216.92	1266.11	1205.68
CN	2068.60	2098.35	2088.08	2108.94	2056.71
CO	2169.80	2148.72	2109.30	2162.13	2098.48
CO^+	2214.20	2214.18	2185.39	2228.25	2164.65
CP	1239.70	1264.31	1263.36	1271.96	1237.42
CS	1285.20	1277.34	1259.25	1290.86	1250.69
N_2	2358.60	2374.48	2334.29	2391.08	2319.63
$N_2{}^+$	2207.00	2270.16	2252.18	2279.75	2220.87
NH	3282.30	3183.72	3189.86	3247.86	3246.85
NF	1141.40	1137.14	1099.68	1137.95	1087.80
NCl	828.00	826.06	812.22	825.33	806.35
NO	1904.20	1901.66	1844.58	1911.17	1838.76
NO^+	2376.40	2389.33	2333.97	2406.85	2322.14
NS	1218.70	1223.24	1195.09	1230.68	1187.40
O_2	1580.20	1565.23	1495.96	1568.15	1494.89
$O_2{}^+$	1904.80	1949.39	1874.42	1958.07	1867.71
OH	3737.80	3622.55	3609.11	3648.88	3630.07
OH^+	3113.40	2992.91	3000.37	3054.84	3062.37
F_2	916.60	1006.95	984.66	1007.99	981.34
$F_2{}^+$	1073.30	1166.73	1132.55	1168.53	1123.55
HF	4138.30	3992.60	3943.92	4005.79	3948.30
HF^+	3090.50	2945.42	2930.07	2983.36	2946.58
Na_2	159.10	159.77	159.33	152.12	164.37
NaH	1172.20	1157.37	1158.70	1178.33	1185.37
NaF	535.70	533.49	528.46	534.62	529.62
NaO	492.30	481.59	478.35	484.31	478.94

(continued)

MgH	1495.20	1426.83	1418.59	1491.76	1515.21
MgH^+	1699.10	1681.72	1686.00	1711.70	1742.35
MgO	784.80	817.05	807.87	815.84	805.42
MgS	528.70	541.32	538.60	541.67	535.72
Al_2	350.00	355.01	359.42	356.04	351.61
AlH	1682.60	1629.37	1603.52	1682.04	1700.58
AlF	802.30	771.53	759.01	776.90	766.18
AlCl	481.30	470.88	465.74	476.30	471.33
AlO	979.20	964.59	953.78	965.69	954.37
AlS	617.10	614.07	611.12	618.05	612.63
Si_2	511.00	554.00	554.40	558.72	493.60
SiH	2041.80	1983.17	1984.50	2044.43	2058.56
SiH^+	2157.20	2097.95	2078.92	2144.42	2162.36
SiF	857.20	829.54	808.72	834.03	812.71
SiCl	535.60	523.20	513.89	527.70	515.45
SiN	1151.40	1164.84	1160.28	1169.33	1139.52
SiO	1241.50	1219.16	1196.84	1227.77	1194.08
SiS	749.60	741.53	732.67	749.27	731.31
P_2	780.80	797.87	791.20	805.83	784.59
$P_2{}^+$	672.20	690.94	685.40	700.45	681.13
PH	2365.20	2314.35	2317.01	2368.74	2386.35
PF	846.80	827.94	801.10	831.54	801.88
PCl	551.40	542.79	528.57	544.09	531.49
PN	1337.20	1358.82	1339.02	1370.51	1328.82
PO	1233.30	1219.51	1189.96	1227.10	1187.64
S_2	725.60	714.98	699.30	718.56	695.82
SO	1149.20	1124.27	1088.74	1128.30	1078.93
Cl_2	559.70	541.26	528.78	542.98	524.89
$Cl_2{}^+$	645.60	630.10	613.29	631.30	617.25
HCl	2990.90	2922.44	2901.09	2953.90	2967.87
HCl^+	2673.70	2583.30	2581.67	2635.95	2689.54
ClF	786.10	764.77	743.62	766.26	741.24
ClO	853.80	849.56	825.53	844.85	819.22
ME		-19.28	-32.28	-2.87	-19.71
MAD		34.27	43.49	24.14	36.22

VIII. SOLID TEST SET RESULTS

Here we provide the solid-by-solid tabulation for the band gaps (21 systems), equilibrium lattice constants and cohesive energies (55 solids), and bulk moduli (44 cubic solids) for *v2-sreg*TM compared with its deorbitalized version *v2-sreg*TM-L (PC_{rep}). Results also are provided for *v2-sreg*TM X plus PBE C and its deorbitalized version *v2-sreg*TM-L X (PC_{rep}) plus PBE C.

TABLE XII. Band Gap (eV) of 21 insulators and semiconductors. Experimental lattice parameters were used with all functionals. Experimental values Exptl. and lattice constants are from Ref. [9].

Solid	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
C	5.50	4.14	4.05	4.42	3.92
Si	1.17	0.63	0.63	0.88	0.55
Ge	0.74	0.39	0.30	0.44	0.24
SiC	2.42	1.46	1.35	1.54	1.37
BN	6.36	4.59	4.40	4.73	4.38
BP	2.10	1.28	1.27	1.50	1.20
AlN	4.90	3.50	3.28	3.52	3.30
AlP	2.50	1.71	1.62	1.84	1.59
AlAs	2.23	1.60	1.49	1.66	1.40
GaN	3.28	1.77	1.45	1.76	1.38
GaP	2.35	1.67	1.58	1.73	1.61
GaAs	1.52	1.00	0.79	1.07	0.80
InP	1.42	0.99	0.76	1.07	0.85
InAs	0.42	0.18	0.00	0.22	0.03
InSb	0.24	0.24	0.11	0.28	0.13
LiH	4.94	3.34	3.27	3.69	3.55
LiF	14.20	9.31	8.83	9.28	8.76
LiCl	9.40	6.79	6.45	6.87	6.51
NaF	11.50	6.32	5.83	6.33	5.83
NaCl	8.50	5.39	5.08	5.48	5.12
MgO	7.83	5.05	4.62	5.05	4.58
ME		-1.53	-1.73	-1.44	-1.73
MAD		1.53	1.73	1.44	1.73

TABLE XIII. Equilibrium lattice constants, $a_0(\AA)$ comparisons of 55 solids. Experimental values Exptl. are from Ref. [7], include zero-point effects.

Solid	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
C	3.553	3.565	3.580	3.560	3.564
Si	5.421	5.430	5.450	5.420	5.432
Ge	5.644	5.700	5.714	5.687	5.696
Sn	6.477	6.559	6.599	6.542	6.576
SiC	4.346	4.353	4.370	4.347	4.361
BN	3.592	3.618	3.623	3.612	3.618
BP	4.525	4.530	4.547	4.523	4.530
AlN	4.368	4.372	4.387	4.366	4.378
AlP	5.451	5.466	5.481	5.456	5.458
AlAs	5.649	5.674	5.688	5.665	5.692
GaN	4.520	4.557	4.576	4.552	4.566
GaP	5.439	5.487	5.516	5.479	5.487
GaAs	5.640	5.690	5.720	5.679	5.718
InP	5.858	5.950	5.978	5.941	5.955
InAs	6.047	6.135	6.166	6.122	6.155
InSb	6.468	6.561	6.601	6.546	6.585
LiH	3.979	3.986	3.984	3.944	3.977
LiF	3.972	3.993	4.008	3.971	3.992
LiCl	5.070	5.082	5.077	5.047	5.048
NaF	4.582	4.501	4.523	4.495	4.524
NaCl	5.569	5.509	5.520	5.495	5.493
MgO	4.189	4.207	4.217	4.200	4.213
Li	3.443	3.434	3.402	3.403	3.392
Na	4.214	4.119	4.116	4.118	4.137
K	5.212	5.207	5.189	5.213	5.192
Rb	5.577	5.559	5.642	5.585	5.594
Cs	6.039	6.063	6.081	6.083	6.021
Ca	5.556	5.475	5.484	5.482	5.497
Ba	5.002	4.999	5.000	5.002	5.049
Sr	6.040	5.988	5.997	5.994	6.043
Al	4.018	3.982	3.997	3.975	3.987
Fe	2.853	2.807	2.811	2.806	2.813
Co	3.524	3.497	3.508	3.500	3.493
Ni	3.508	3.479	3.484	3.473	3.483
Sc	3.270	3.235	3.231	3.234	3.238
Y	3.594	3.593	3.606	3.595	3.598
Ti	2.915	2.879	2.883	2.877	2.888
Zr	3.198	3.206	3.222	3.205	3.219
Hf	3.151	3.134	3.163	3.132	3.166
V	3.021	2.966	2.971	2.963	2.974
Nb	3.294	3.318	3.329	3.317	3.328
Ta	3.299	3.287	3.311	3.284	3.312
Mo	3.141	3.141	3.154	3.138	3.156
W	3.160	3.154	3.171	3.151	3.173
Tc	2.716	2.713	2.726	2.710	2.726
Re	2.744	2.749	2.761	2.747	2.761
Ru	2.669	2.673	2.684	2.670	2.683
Os	2.699	2.706	2.721	2.704	2.720
Rh	3.794	3.806	3.815	3.801	3.815
Ir	3.831	3.850	3.867	3.846	3.866
Pd	3.876	3.909	3.917	3.903	3.913
Pt	3.913	3.941	3.959	3.935	3.957
Cu	3.595	3.577	3.584	3.570	3.584
Ag	4.062	4.092	4.101	4.084	4.094
Au	4.062	4.118	4.134	4.111	4.127
ME		0.004	0.018	-0.002	0.012
MAD		0.031	0.041	0.029	0.035

TABLE XIV. Cohesive energies, $E_{coh}(eV/atom)$ of 55 solids. Experimental values Exptl. are from Ref. [7], include zero-point effects.

Solid	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
C	7.550	7.528	7.318	7.527	7.492
Si	4.680	4.642	4.497	4.696	4.525
Ge	3.890	3.889	3.744	3.912	3.815
Sn	3.160	3.356	3.273	3.377	3.346
SiC	6.480	6.462	6.211	6.465	6.302
BN	6.760	6.906	6.745	6.894	6.822
BP	5.140	5.277	5.085	5.302	5.201
AlN	5.850	5.922	5.770	5.920	5.828
AlP	4.320	4.270	4.143	4.308	4.132
AlAs	3.820	3.874	3.748	3.886	3.733
GaN	4.550	4.620	4.475	4.637	4.540
GaP	3.610	3.685	3.523	3.715	3.584
GaAs	3.340	3.372	3.203	3.395	3.236
InP	3.470	3.348	3.231	3.371	3.276
InAs	3.080	3.114	2.992	3.135	3.020
InSb	2.810	2.830	2.813	2.850	2.838
LiH	2.490	2.447	2.454	2.470	2.518
LiF	4.460	4.388	4.246	4.339	4.359
LiCl	3.590	3.516	3.381	3.469	3.477
NaF	3.970	3.970	3.815	3.927	3.957
NaCl	3.340	3.291	3.144	3.260	3.272
MgO	5.200	5.177	5.094	5.192	5.156
Li	1.670	1.641	1.635	1.595	1.664
Na	1.120	1.134	1.103	1.118	1.187
K	0.940	0.954	0.937	0.952	1.026
Rb	0.860	0.849	0.858	0.868	0.936
Cs	0.810	0.803	0.662	0.812	2.241
Ca	1.870	1.923	2.007	2.052	2.057
Ba	1.910	1.947	1.972	2.078	2.021
Sr	1.730	1.835	1.785	1.981	1.845
Al	3.430	3.656	3.522	3.667	3.661
Fe	4.300	5.121	4.925	5.166	5.294
Co	4.420	5.242	4.910	5.360	5.478
Ni	4.480	5.132	5.793	5.193	5.159
Sc	3.930	4.337	4.187	4.410	4.383
Y	4.390	4.386	4.142	4.505	4.338
Ti	4.880	5.364	5.248	5.372	5.649
Zr	6.270	6.001	5.463	6.049	5.538
Hf	6.460	6.854	6.503	6.994	6.641
V	5.350	5.606	5.596	5.623	5.740
Nb	7.600	7.168	7.090	7.204	7.218
Ta	8.130	8.807	8.383	8.942	8.551
Mo	6.860	6.676	6.755	6.720	6.693
W	8.940	9.017	8.723	9.090	8.751
Tc	6.880	7.299	7.135	7.360	7.285
Re	8.050	8.440	8.108	8.568	8.224
Ru	6.770	6.954	6.779	6.987	7.143
Os	8.200	8.872	8.486	8.994	8.621
Rh	5.780	6.050	5.747	6.085	6.115
Ir	6.990	7.783	7.329	7.851	7.550
Pd	3.930	4.470	4.314	4.524	4.389
Pt	5.870	6.130	5.752	6.212	5.896
Cu	3.510	4.198	3.995	4.262	4.037
Ag	2.960	3.168	3.009	3.217	3.065
Au	3.830	3.702	3.464	3.764	3.567
ME		0.159	0.010	0.199	0.140
MAD		0.216	0.205	0.251	0.260

TABLE XV. Bulk modulus, $B_0(GPa)$ of 44 cubic solids. Experimental values Exptl. are from Ref. [8], these values were obtained by subtracting the zero-point phonon effect from the experimental zero-temperature values.

Solid	Exptl.	*v2-sreg*TM X *rreg*TM C	*v2-sreg*TM-L X *rreg*TM-L C	*v2-sreg*TM X *PBE* C	*v2-sreg*TM-L X *PBE* C
C	454.700	439.805	416.340	449.531	431.241
Si	101.300	95.389	91.708	100.463	93.979
Ge	79.400	69.611	65.360	71.784	70.593
Sn	42.800	42.673	42.403	43.929	70.979
SiC	229.100	224.220	214.309	228.388	209.223
BN	410.200	383.296	375.576	390.743	382.044
BP	168.000	166.357	160.835	171.680	164.986
AlN	206.000	207.037	194.185	210.108	202.650
AlP	87.400	89.942	84.686	93.076	91.287
AlAs	75.000	75.557	72.567	77.566	83.135
GaN	213.000	198.521	186.559	201.514	195.052
GaP	89.600	87.463	80.747	89.785	80.337
GaAs	76.700	71.990	66.138	73.764	78.644
InP	72.000	68.256	66.662	69.924	65.454
InAs	58.600	57.289	60.371	58.661	46.961
InSb	46.100	43.221	42.562	44.299	43.357
LiH	40.100	37.481	38.331	40.751	41.783
LiF	76.300	78.996	77.549	82.599	81.111
LiCl	38.700	36.717	35.848	38.798	37.835
NaF	53.100	59.873	59.184	60.157	59.567
NaCl	27.600	31.063	31.554	31.492	26.840
MgO	169.800	165.926	160.719	167.910	159.019
Li	13.100	13.909	16.494	14.662	17.932
Na	7.900	8.807	8.549	8.830	7.747
K	3.800	4.196	4.806	3.943	14.176
Rb	3.600	3.421	5.306	3.256	3.846
Cs	2.300	2.187	2.826	2.151	8.155
Ca	15.900	20.742	19.048	18.814	19.334
Ba	10.600	9.440	9.497	9.369	8.905
Sr	12.000	12.093	13.281	13.053	11.769
Al	77.100	91.171	85.461	93.144	92.646
Ni	192.500	223.348	221.831	226.624	227.568
V	165.800	200.526	201.059	202.116	199.661
Nb	173.200	179.238	174.747	180.736	176.274
Ta	202.700	211.184	208.630	212.688	208.336
Mo	276.200	277.833	275.092	279.859	277.175
W	327.500	328.582	323.924	331.325	321.185
Rh	277.100	277.697	275.645	281.255	279.400
Ir	362.200	373.459	361.476	378.318	362.796
Pd	187.200	189.957	186.423	193.530	189.626
Pt	285.500	271.130	263.303	275.772	267.805
Cu	144.300	153.997	159.147	160.709	163.448
Ag	105.700	110.540	106.258	113.239	110.119
Au	182.000	159.380	153.057	163.612	158.542
ME		0.223	-3.265	2.732	-0.027
MAD		6.602	8.747	6.542	9.249

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