Supporting Information: Reworking the Tao–Mo exchange-correlation functional: III. Improved De-orbitalization strategy and faithful de-orbitalization

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Abstract

We provide detailed, system-by-system tabulation of the numerical results of test calculations against standard molecular and crystalline system data sets.

We also provide detailed data from the $3d$ elememtal magnetiztion calculations.

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Molecular Test Set Results

Here we provide the molecule-by-molecule tabulation for the G3/99, T96R, and T82-F test sets for different versions of *sr*TM-L$\tilde{q}$ compared with the experimental values.

Table S1: Standard enthalpies of formation (ΔH_f) in kcal/mol for the G3X/99 molecular test set[S1,S2] obtained with different approximate exchange-correlation functionals.

Molecule	Exptl.	*sr*TM-L$\tilde{q}$			
		PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
LiH	33.30	36.385	36.401	36.906	36.922
^{2}BeH	81.70	74.040	74.002	74.388	74.347
^{2}CH	142.50	143.191	143.179	142.797	142.841
CH_2 ($^3B_1$)	93.60	85.570	85.746	87.393	87.737
CH_2 ($^1A_1$)	102.60	107.278	107.269	107.735	107.822
$^3CH_3$	35.00	28.794	28.909	30.722	31.101
CH_4	-17.80	-17.654	-17.401	-13.651	-13.022
^{3}NH	85.80	81.517	81.608	78.182	78.113
NH_2 ($^2B_1$)	44.50	39.797	39.857	36.227	36.215
NH_3	-10.90	-10.964	-10.828	-10.779	-10.393
^{2}OH	9.00	5.965	6.013	4.962	4.941
H_2O	-57.80	-56.832	-56.660	-54.058	-53.690
HF	-65.20	-63.535	-63.398	-59.140	-58.788
SiH_2 ($^1A_1$)	65.20	69.259	69.366	69.171	69.293
SiH_2 ($^3B_1$)	86.20	79.406	79.586	80.362	80.560
$^2SiH_3$	47.90	45.436	45.648	46.511	46.747
SiH_4	8.20	12.520	12.764	13.504	13.763
$^2PH_2$	33.10	32.623	32.754	31.370	31.519

(continued)

PH_3	1.30	7.077	7.299	6.116	6.364
H_2S	-4.90	-2.147	-1.948	-0.881	-0.522
HCl	-22.00	-20.643	-20.511	-19.313	-19.012
Li_2	51.60	56.370	56.439	56.569	56.639
LiF	-80.10	-76.822	-76.824	-73.324	-73.086
HC≡CH	54.60	51.040	51.396	53.330	54.322
$H_2C{=}CH_2$	12.50	8.516	8.983	14.080	15.259
$H_3C{-}CH_3$	-20.10	-21.275	-20.554	-14.112	-12.674
CN	105.20	99.774	100.316	97.152	97.634
HCN	30.90	28.892	29.358	27.792	28.433
CO	-26.40	-25.895	-25.362	-23.753	-23.107
^{2}HCO	10.00	1.877	2.467	3.337	3.967
H_2CO	-26.10	-29.200	-28.532	-26.637	-25.912
CH_3OH	-48.00	-48.822	-48.205	-44.531	-43.623
N_2	0.00	1.829	2.480	-2.959	-2.567
H_2NNH_2	23.30	23.587	24.120	21.724	22.423
NO	21.80	17.211	17.937	13.126	13.385
$^3O_2$	0.00	-11.950	-11.388	-13.867	-13.646
H_2O_2	-32.40	-37.331	-37.055	-36.834	-36.537
F_2	0.00	-5.309	-5.136	-4.654	-4.569
CO_2	-94.00	-103.778	-102.356	-100.203	-98.937
Na_2	34.00	34.458	34.584	34.063	34.199
Si_2	139.90	138.610	138.890	135.236	135.610
P_2	34.30	43.535	44.034	39.409	39.992
$^3S_2$	30.70	24.873	25.572	25.537	26.127

(continued)

Cl_2	0.00	0.070	0.403	0.436	0.785
NaCl	-43.60	-40.233	-40.105	-39.581	-39.373
SiO	-24.60	-21.640	-21.520	-21.214	-21.024
CS	66.90	68.599	69.077	69.598	70.316
SO	1.20	-6.378	-5.892	-6.158	-5.837
ClO	24.30	17.518	17.902	15.459	15.603
ClF	-13.30	-14.989	-14.752	-13.413	-13.151
Si_2H_6	19.10	23.870	24.408	25.508	26.161
CH_3Cl	-19.60	-19.999	-19.439	-16.906	-16.060
H_3C-SH	-5.50	-4.577	-3.907	-0.722	0.357
HOCl	-18.40	-20.509	-20.186	-19.987	-19.651
SO_2	-71.00	-72.391	-71.248	-71.274	-70.386
BF_3	-271.40	-274.365	-273.747	-260.552	-259.222
BCl_3	-96.30	-102.443	-101.422	-97.739	-96.237
AlF_3	-289.00	-286.147	-285.780	-274.453	-273.305
$AlCl_3$	-139.70	-142.716	-142.031	-138.356	-137.279
CF_4	-223.10	-225.902	-224.079	-213.843	-211.646
CCl_4	-22.90	-26.605	-24.743	-24.143	-22.067
OCS	-33.10	-43.371	-42.127	-40.410	-39.119
CS_2	28.00	18.816	19.938	21.311	22.712
F_2CO	-145.00	-151.620	-150.067	-144.122	-142.465
SiF_4	-386.00	-378.093	-377.363	-361.928	-360.180
$SiCl_4$	-158.40	-156.906	-155.540	-151.871	-150.056
NNO	19.70	8.221	9.936	1.841	2.705
ClNO	12.60	-0.034	0.944	-4.143	-3.602

(continued)

NF_3	-31.60	-47.202	-46.398	-46.606	-45.748
PF_3	-229.10	-222.247	-221.736	-215.189	-214.107
O_3	33.90	22.223	23.031	17.152	17.409
F_2O	5.90	-7.959	-7.606	-8.641	-8.452
ClF_3	-38.00	-58.226	-57.637	-53.522	-52.605
$F_2C{=}CF_2$	-161.30	-172.221	-170.409	-159.135	-156.571
$Cl_2C{=}CCl_2$	-5.50	-13.125	-10.680	-8.439	-5.486
$F_3C{-}CN$	-118.40	-128.333	-126.394	-120.173	-117.617
$HC{\equiv}C{-}CH_3$	44.40	37.678	38.516	44.026	45.901
$H_2C{=}C{=}CH_2$	45.40	33.826	34.588	41.091	42.972
C_3H_4 (cyclopropene)	67.80	59.453	60.680	64.828	66.738
$H_2C{=}CH{-}CH_3$	4.80	-1.245	-0.281	7.922	9.985
C_3H_6 (cyclopropane)	12.80	7.941	9.392	15.628	17.824
$CH_3{-}CH_2{-}CH_3$	-25.10	-27.604	-26.384	-17.177	-14.885
C_4H_6 (Z-1,3-butadiene)	26.40	14.762	15.948	25.888	28.557
C_4H_6 (2-butyne)	34.80	26.194	27.530	36.412	39.174
C_4H_6 (methylenecyclopropane)	47.90	34.959	36.634	44.890	47.732
C_4H_6 (bicyclo[1.1.0]butane)	51.90	44.733	46.956	52.579	55.524
C_4H_6 (cyclobutene)	38.20	28.964	30.493	39.398	42.247
C_4H_8 (cyclobutane)	6.60	0.014	1.774	12.146	15.235
C_4H_8 (isobutene)	-4.10	-11.710	-10.227	0.971	3.944
C_4H_{10} (trans butane)	-30.10	-33.736	-32.010	-20.214	-17.066
C_4H_{10} (isobutane)	-32.20	-35.863	-34.117	-22.178	-18.992
C_5H_8 (spiropentane)	44.30	33.597	36.268	45.527	49.345
C_6H_6 (benzene)	19.90	-1.982	0.180	15.269	19.704

(continued)

CH_2F_2	-107.70	-108.832	-108.087	-102.034	-100.951
CHF_3	-166.30	-168.442	-167.204	-159.200	-157.608
CH_2Cl_2	-22.60	-23.683	-22.723	-21.015	-19.816
$CHCl_3$	-24.50	-26.594	-25.189	-24.048	-22.420
CH_3NH_2	-5.20	1.078	1.776	3.853	4.926
CH_3CN	18.00	12.488	13.428	15.275	16.769
CH_3NO_2 (nitromethane)	-17.90	-30.869	-28.876	-32.193	-30.620
CH_3ONO (methyl nitrite)	-16.10	-27.995	-26.426	-29.922	-28.646
CH_3SiH_3	-7.00	-3.702	-3.129	0.730	1.769
HCO_2H	-90.40	-96.484	-95.281	-92.356	-91.078
HCO_2CH_3	-85.50	-92.907	-91.272	-87.423	-85.616
CH_3CONH_2	-57.00	-66.113	-64.482	-60.010	-57.721
C_2H_5N (aziridine)	30.20	25.096	26.396	27.715	29.383
NCCN (cyanogen)	74.10	60.791	61.830	59.865	61.461
$NH(CH_3)_2$	-4.30	-6.616	-5.360	-1.458	0.385
$CH_3CH_2NH_2$	-11.30	-14.914	-13.757	-9.023	-7.084
$H_2C{=}C{=}O$ (ketene)	-11.60	-23.494	-22.405	-18.314	-16.766
C_2H_4O (oxirane)	-12.60	-17.699	-16.656	-14.074	-12.724
CH_3CHO	-39.50	-45.318	-44.183	-38.950	-37.336
$O{=}CH{-}CH{=}O$	-50.80	-60.337	-58.847	-55.358	-53.665
CH_3CH_2OH	-56.10	-58.655	-57.564	-50.999	-49.231
$(CH_3)_2O$	-44.00	-45.995	-44.863	-40.175	-38.665
C_2H_4S (thiooxirane)	19.60	15.636	16.942	20.235	21.935
$(CH_3)_2S{=}O$	-36.20	-40.570	-38.828	-33.049	-30.735
CH_3CH_2SH	-11.10	-11.290	-10.128	-4.225	-2.300

(continued)

$(CH_3)_2S$	-8.90	-9.963	-8.779	-3.395	-1.544
$H_2C{=}CHF$	-34.00	-39.857	-39.107	-32.754	-31.289
CH_3CH_2Cl	-26.60	-28.775	-27.748	-22.394	-20.707
$H_2C{=}CHCl$	5.20	-0.110	0.795	4.970	6.536
$H_2C{=}CHCN$	43.20	33.732	34.865	38.554	40.646
$(CH_3)_2C{=}O$	-51.70	-59.525	-57.908	-49.495	-46.993
CH_3CO_2H	-103.40	-111.119	-109.449	-103.310	-101.153
CH_3CFO	-105.70	-112.654	-111.165	-104.128	-102.118
CH_3COCl	-57.70	-67.198	-65.678	-61.045	-59.060
$CH_3CH_2CH_2Cl$	-31.50	-34.873	-33.339	-25.398	-22.862
$(CH_3)_2CHOH$	-65.20	-69.658	-68.059	-58.539	-55.875
$CH_3{-}O{-}CH_2CH_3$	-51.70	-55.694	-54.084	-46.505	-44.136
$(CH_3)_3N$	-6.60	-9.582	-7.686	-1.978	0.668
C_4H_4O (furan)	-8.30	-23.349	-21.393	-13.740	-10.675
C_4H_4S (thiophene)	27.50	14.135	16.229	24.516	28.021
C_4H_5N (pyrrole)	25.90	9.677	11.770	18.641	22.047
C_5H_5N (pyridine)	33.60	12.329	14.665	24.406	28.422
H_2	0.00	2.116	2.122	2.738	2.744
^2SH	34.20	33.728	33.817	33.959	34.099
$^2C{\equiv}CH$	135.80	128.390	128.822	129.526	130.379
'HC=CH_2 ($^2A''$)'	71.00	60.504	60.938	64.172	65.172
'$CH_3C{=}O$ ($^2A''$)'	-2.40	-13.825	-12.800	-8.720	-7.311
$CH_2{-}OH$ (^2A)	-4.00	-12.638	-12.159	-9.056	-8.290
'CH_3O ($^2A''$)'	5.20	-2.911	-2.376	-1.414	-0.803
'CH_3CH_2O ($^2A''''$)'	-2.90	-13.543	-12.535	-8.615	-7.144

(continued)

'CH_3S ($^2A''$)'	29.80	25.760	26.324	28.842	29.714
'CH_2CH_3 ($^2A''$)'	28.60	19.955	20.542	25.494	26.685
'$(CH_3)_2CH$ ($^2A''$)'	21.10	9.901	10.992	19.062	21.093
$^2C(CH_3)_3$	12.00	-0.764	0.864	11.926	14.821
NO_2 ($^2A_1$)	8.10	-8.584	-7.119	-13.721	-13.034
$CH_3CH{=}C{=}CH_2$	38.80	25.869	27.116	36.661	39.398
C_5H_8 (isoprene)	18.00	4.922	6.632	19.468	23.045
C_5H_{10} (cyclopentane twist)	-18.50	-24.886	-22.526	-8.915	-4.832
C_5H_{12} (n-pentane)	-35.00	-39.768	-37.541	-23.182	-19.178
$C(CH_3)_4$ (neopentane)	-40.10	-45.263	-42.969	-28.346	-24.239
C_6H_8 (1,3-cyclohexadiene)	25.40	10.751	13.113	28.026	32.594
C_6H_8 (1,4-cyclohexadiene)	25.00	11.466	13.835	28.819	33.405
C_6H_{12} (cyclohexane chair)	-29.40	-35.942	-33.034	-16.758	-11.746
C_6H_{14} (n-hexane)	-39.90	-46.286	-43.565	-26.112	-21.247
C_6H_{14} (3-methylpentane)	-41.10	-46.525	-43.764	-26.833	-21.936
$C_6H_5{-}CH_3$ (toluene)	12.00	-11.092	-8.405	9.623	14.963
C_7H_{16} (n-heptane)	-44.80	-52.016	-48.788	-29.138	-23.422
C_8H_8 (cyclooctatetraene)	70.70	45.893	48.676	68.019	73.870
C_8H_{18} (n-octane)	-49.80	-58.157	-54.427	-32.118	-25.546
$C_{10}H_8$ (naphtalene)	35.90	-3.303	0.561	25.252	32.960
$C_{10}H_8$ (azulene)	69.10	27.587	31.363	56.037	63.639
$CH_3CO_2CH_3$ (Z-methylacetate)	-98.40	-106.982	-104.866	-97.857	-95.165
$(CH_3)_3COH$ (t-butanol)	-74.70	-80.821	-78.696	-66.327	-62.745
$C_6H_5NH_2$ (aniline)	20.80	-4.909	-2.223	11.782	16.867
C_6H_5OH (phenol)	-22.30	-46.906	-44.234	-28.708	-23.782

(continued)

C_4H_6O (divinyl ether)	-3.30	-16.303	-14.565	-5.960	-3.058
C_4H_8O (tetrahydrofuran)	-44.00	-49.433	-47.222	-37.857	-34.571
C_5H_8O (cyclopentanone)	-45.90	-57.908	-55.122	-42.391	-38.070
$C_6H_4O_2$ (benzoquinone)	-29.40	-55.359	-52.352	-39.181	-34.337
$C_6H_4N_2$ (pyrimidine)	46.80	24.833	27.345	31.935	35.556
$(CH_3)_2SO_2$	-89.20	-93.215	-90.679	-83.516	-80.521
C_6H_5Cl (chlorobenzene)	12.50	-10.741	-8.133	6.163	11.007
$NC(CH_2)_2CN$ (succinonitrile)	50.10	38.526	40.629	43.312	46.511
$C_4H_4N_2$ (pyrazine)	46.90	28.413	30.907	35.378	38.970
C_4H_4O (3-butyn-2-one)	15.60	4.521	6.187	13.233	16.120
C_4H_6O (E-crotonaldehyde)	-24.00	-38.260	-36.413	-26.479	-23.394
$C_4H_6O_3$ (acetic anhydride)	-136.80	-153.383	-150.248	-140.653	-136.768
C_4H_6S (2,5-dihydrothiophene)	20.80	12.041	14.105	23.149	26.586
$(CH_3)_2CHCN$	5.60	-0.562	1.361	8.504	11.678
C_4H_8O (methyl ethyl ketone)	-57.10	-65.941	-63.819	-52.909	-49.557
$(CH_3)_2CHCHO$	-51.60	-58.460	-56.304	-45.805	-42.481
$C_4H_8O_2$ (1,4-dioxane)	-75.50	-82.813	-80.220	-72.190	-68.779
C_4H_8S (tetrahydrothiophene)	-8.20	-12.195	-9.865	-0.125	3.514
$(CH_3)_3CCl$	-43.50	-49.317	-47.272	-36.280	-32.807
C_4H_9Cl (n-butyl chloride)	-37.00	-41.082	-39.053	-28.275	-24.885
C_4H_9N (tetrahydropyrrole)	-0.80	-7.384	-5.026	3.405	7.027
$C_4H_9NO_2$ (2-nitrobutane)	-39.10	-55.445	-51.954	-47.244	-43.110
$(CH_3CH_2)_2O$	-60.30	-65.445	-63.365	-52.694	-49.463
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	-93.10	-99.279	-96.768	-87.799	-84.436
$(CH_3)_3CSH$	-26.20	-29.842	-27.616	-16.310	-12.581

(continued)

$C_4H_{10}S_2$ (diethyl disulfide)	-17.90	-20.608	-17.988	-7.991	-4.043
$(CH_3)_3CNH_2$	-28.90	-35.087	-32.884	-22.455	-18.700
$(CH_3)_4Si$	-55.70	-54.855	-53.250	-40.203	-36.767
C_5H_6S (2-methyl thiophene)	20.00	5.222	7.811	19.036	23.418
C_5H_7N (N-methyl pyrrole)	24.60	7.912	10.602	19.377	23.529
$C_5H_{10}O$ (tetrahydropyran)	-53.40	-60.087	-57.330	-45.160	-40.940
$(CH_3CH_2)_2C{=}O$	-61.60	-72.271	-69.649	-56.233	-52.031
$C_5H_{10}O_2$ (isopropyl acetate)	-115.10	-127.029	-123.948	-110.912	-106.482
$C_5H_{10}S$ (tetrahydrothiopyran)	-15.20	-20.174	-17.313	-4.863	-0.299
$C_5H_{11}N$ (piperidine)	-11.30	-18.040	-15.124	-3.915	0.638
$C_5H_{12}O$ (t-butyl methyl ether)	-67.80	-74.543	-71.926	-58.721	-54.563
$C_6H_4F_2$ (1,3-difluorobenzene)	-73.90	-99.862	-97.138	-79.463	-74.405
$C_6H_4F_2$ (1,4-difluorobenzene)	-73.30	-99.157	-96.457	-78.750	-73.703
C_6H_5F (fluorobenzene)	-27.40	-51.252	-48.814	-32.449	-27.707
$C_6H_{14}O$ (diisopropyl ether)	-76.30	-84.411	-81.353	-64.963	-59.975
PF_5	-381.10	-374.329	-373.006	-358.880	-356.655
SF_6	-291.70	-298.171	-295.823	-282.865	-279.932
P_4	14.10	25.231	27.228	15.370	16.845
SO_3	-94.60	-99.832	-97.720	-98.304	-96.800
SCl_2	-4.20	-5.030	-4.289	-4.741	-3.993
$POCl_3$	-133.80	-133.003	-131.146	-131.008	-129.137
PCl_5	-86.10	-90.874	-88.636	-90.144	-87.855
Cl_2O_2S	-84.80	-91.731	-89.472	-89.086	-87.125
PCl_3	-69.00	-67.573	-66.369	-68.295	-67.106
Cl_2S_2	-4.00	-11.308	-10.120	-11.224	-10.036

(continued)

$SiCl_2$ ($^1A_1$)	-40.30	-38.714	-38.150	-37.429	-36.748
CF_3Cl	-169.70	-174.419	-172.593	-164.981	-162.844
C_2F_6	-320.90	-329.442	-326.645	-311.276	-307.707
$^2CF_3$	-111.80	-123.217	-122.133	-113.602	-112.140
$^2C_6H_5$ (phenyl radical)	80.50	51.568	53.707	66.657	70.854
ME		-6.815	-5.416	0.313	2.451
MAD		7.864	6.647	5.770	6.265

Table S2: Bond lengths in Å for the T96-R molecular test set[S3,S4] from different approximate XC functionals.

		$srTM\text{-}L\tilde{q}$			
Molecule	Exptl.	PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
H_2	0.741	0.745	0.745	0.746	0.746
Li_2	2.673	2.714	2.715	2.717	2.718
LiH	1.595	1.595	1.595	1.600	1.600
LiF	1.564	1.564	1.564	1.570	1.570
LiCl	2.021	2.015	2.015	2.015	2.016
LiO	1.688	1.688	1.688	1.692	1.692
Be_2	2.440	2.414	2.415	2.429	2.428
BeH	1.343	1.352	1.352	1.354	1.354
BeF	1.361	1.368	1.369	1.374	1.375
BeO	1.331	1.331	1.331	1.337	1.337
BeS	1.742	1.742	1.742	1.744	1.744

(continued)

B_2	1.590	1.606	1.606	1.609	1.611
BH	1.232	1.242	1.242	1.244	1.244
BF	1.263	1.264	1.264	1.272	1.273
BF_3	1.313	1.312	1.312	1.320	1.321
BCl	1.715	1.715	1.715	1.725	1.726
BCl_3	1.742	1.735	1.736	1.741	1.742
BN	1.281	1.320	1.320	1.323	1.324
BO	1.204	1.203	1.203	1.210	1.210
BS	1.609	1.605	1.604	1.610	1.610
C_2	1.242	1.388	1.388	1.393	1.393
CH	1.120	1.125	1.125	1.129	1.129
CH_4	1.087	1.088	1.088	1.091	1.091
CF	1.272	1.278	1.279	1.291	1.293
CF_4	1.323	1.327	1.328	1.337	1.338
CCl	1.645	1.648	1.649	1.660	1.663
CCl_4	1.767	1.775	1.777	1.783	1.786
CN	1.172	1.163	1.163	1.167	1.168
CO	1.128	1.126	1.126	1.133	1.134
CO^+	1.115	1.111	1.111	1.118	1.118
CO_2	1.160	1.161	1.161	1.170	1.170
CP	1.562	1.551	1.551	1.553	1.554
CS	1.535	1.530	1.530	1.539	1.539
CS_2	1.553	1.546	1.546	1.555	1.556
N_2	1.098	1.093	1.093	1.099	1.100
N_2^+	1.116	1.105	1.105	1.109	1.110

(continued)

NH	1.036	1.043	1.043	1.048	1.049
NH^+	1.070	1.080	1.080	1.084	1.084
NF	1.317	1.322	1.324	1.338	1.340
NCl	1.611	1.612	1.614	1.626	1.629
NO	1.151	1.150	1.150	1.159	1.160
NO^+	1.063	1.060	1.061	1.067	1.068
NS	1.494	1.491	1.491	1.501	1.503
O_2	1.208	1.213	1.215	1.226	1.228
$O_2{}^+$	1.116	1.116	1.117	1.125	1.126
OH	0.970	0.974	0.975	0.978	0.978
OH^+	1.029	1.040	1.040	1.043	1.043
OF	1.358	1.359	1.360	1.372	1.374
F_2	1.412	1.411	1.412	1.424	1.425
$F_2{}^+$	1.322	1.315	1.316	1.326	1.327
HF	0.917	0.922	0.922	0.928	0.928
HF^+	1.001	1.013	1.013	1.016	1.016
Na_2	3.079	3.079	3.079	3.079	3.079
NaH	1.887	1.887	1.887	1.887	1.887
NaF	1.926	1.921	1.921	1.928	1.930
NaCl	2.361	2.352	2.353	2.353	2.354
NaO	2.052	2.048	2.049	2.052	2.055
MgH	1.730	1.742	1.742	1.747	1.747
MgF	1.750	1.762	1.762	1.770	1.771
MgCl	2.196	2.203	2.204	2.206	2.207
MgO	1.748	1.731	1.731	1.738	1.739

(continued)

Al_2	2.466	2.449	2.450	2.454	2.456
AlH	1.648	1.659	1.660	1.666	1.666
AlF	1.654	1.663	1.664	1.672	1.673
AlCl	2.130	2.138	2.139	2.144	2.146
AlO	1.618	1.614	1.614	1.623	1.624
AlS	2.029	2.029	2.029	2.032	2.033
Si_2	2.246	2.146	2.146	2.271	2.272
SiH	1.520	1.529	1.529	1.535	1.535
SiH_4	1.480	1.480	1.480	1.484	1.484
SiF	1.601	1.613	1.613	1.623	1.624
SiF_4	1.553	1.560	1.561	1.570	1.571
SiCl	2.058	2.063	2.063	2.073	2.075
$SiCl_4$	2.019	2.017	2.017	2.023	2.024
SiN	1.572	1.563	1.564	1.566	1.567
SiO	1.510	1.513	1.513	1.521	1.522
SiS	1.929	1.931	1.930	1.937	1.937
P_2	1.893	1.885	1.884	1.891	1.892
P_4	2.210	2.192	2.194	2.196	2.199
PH	1.421	1.427	1.427	1.435	1.435
PF	1.589	1.601	1.602	1.614	1.615
PCl	2.015	2.015	2.017	2.029	2.032
PN	1.491	1.484	1.484	1.491	1.492
PO	1.476	1.480	1.480	1.490	1.491
S_2	1.889	1.894	1.896	1.902	1.904
SH	1.341	1.344	1.344	1.348	1.348

(continued)

SF	1.601	1.613	1.614	1.626	1.627
SF_6	1.561	1.579	1.580	1.594	1.596
SO	1.481	1.489	1.490	1.502	1.504
SO_3	1.420	1.429	1.430	1.441	1.443
Cl_2	1.988	2.005	2.008	2.015	2.017
Cl_2^+	1.891	1.908	1.911	1.915	1.918
HCl	1.275	1.278	1.278	1.281	1.281
HCl^+	1.315	1.322	1.322	1.325	1.326
ClF	1.628	1.648	1.649	1.661	1.663
ClO	1.570	1.580	1.583	1.595	1.597
ME		0.003	0.004	0.011	0.012
MAD		0.010	0.010	0.013	0.014

Table S3: Harmonic vibrational frequencies in cm^{-1} for the T82-F molecular test set[S3,S4] obtained with different approximate exchange-correlation functionals.

		srTM-L$\tilde{q}$			
Molecule	Exptl.	PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
H_2	4401.20	4395.56	4395.46	4383.09	4382.83
Li_2	351.40	333.41	334.37	337.23	336.09
LiH	1405.70	1403.86	1405.21	1389.72	1388.62
LiF	910.60	910.49	910.12	900.79	898.89
LiCl	643.00	649.59	649.19	649.90	648.64
LiO	814.60	811.86	811.63	807.50	806.57
LiNa	256.80	249.16	248.68	250.59	249.98
Be_2	267.90	359.23	353.54	344.83	343.34
BeH	2060.80	2020.15	2019.92	1992.34	1992.26
BeH^+	2221.70	2175.33	2173.48	2158.76	2158.50
BeF	1247.40	1235.16	1233.90	1216.38	1213.93
BeCl	846.70	829.17	828.60	824.21	822.49
BeO	1487.30	1512.26	1511.87	1489.15	1486.13
BeS	997.90	1011.22	1011.00	1007.03	1004.73
B_2	1051.30	1031.63	1027.02	1024.73	1021.44
BH	2366.90	2327.74	2326.23	2282.11	2281.93
BF	1402.10	1398.68	1397.47	1365.64	1362.94
BCl	840.30	840.09	837.97	813.87	809.81
BN	1514.60	1567.37	1567.59	1558.18	1556.97
BO	1885.70	1901.40	1901.13	1859.93	1856.12
BS	1180.20	1197.26	1199.57	1184.71	1180.31
C_2	1854.70	1901.34	1897.83	1884.92	1873.58

(continued)

CH	2858.50	2817.67	2819.31	2755.35	2755.40
CF	1308.10	1279.50	1275.49	1224.69	1219.72
CN	2068.60	2140.78	2136.38	2118.34	2112.34
CO	2169.80	2183.33	2181.42	2132.30	2127.21
CO^+	2214.20	2268.09	2265.01	2219.54	2213.01
CP	1239.70	1279.38	1276.27	1281.37	1277.75
CS	1285.20	1300.84	1301.99	1275.63	1270.77
N_2	2358.60	2405.42	2402.67	2360.00	2353.31
N_2^+	2207.00	2309.45	2302.77	2277.75	2270.32
NH	3282.30	3206.01	3202.93	3197.34	3193.08
NF	1141.40	1131.62	1129.45	1122.62	1120.00
NCl	828.00	832.04	825.83	819.26	815.72
NO	1904.20	1912.65	1904.11	1862.29	1853.86
NO^+	2376.40	2410.27	2404.13	2359.19	2351.31
NS	1218.70	1239.15	1234.83	1214.99	1210.22
O_2	1580.20	1566.23	1559.54	1515.41	1509.29
O_2^+	1904.80	1940.37	1929.69	1893.41	1883.70
OH	3737.80	3683.60	3681.40	3659.68	3654.14
OH^+	3113.40	2997.37	2995.04	3002.74	3000.01
F_2	916.60	1014.56	1014.29	989.31	987.93
F_2^+	1073.30	1163.20	1162.61	1137.46	1137.41
HF	4138.30	4067.26	4063.16	3984.27	3975.09
HF^+	3090.50	2993.47	2991.29	2969.12	2965.37
Na_2	159.10	156.82	156.23	159.92	159.52
NaH	1172.20	1159.55	1158.97	1160.89	1160.34

(continued)

NaF	535.70	538.00	537.14	530.43	529.21
NaO	492.30	485.64	485.02	485.19	482.28
MgH	1495.20	1441.63	1440.54	1427.21	1426.26
MgH^+	1699.10	1696.76	1696.77	1690.87	1690.43
MgO	784.80	832.46	831.70	822.71	820.87
MgS	528.70	552.75	552.04	547.01	545.47
Al_2	350.00	365.92	363.64	362.40	360.16
AlH	1682.60	1631.54	1630.55	1602.65	1598.37
AlF	802.30	779.98	778.81	767.16	765.28
AlCl	481.30	478.98	478.04	471.31	469.70
AlO	979.20	996.88	995.69	977.35	974.84
AlS	617.10	620.26	617.85	621.09	618.81
Si_2	511.00	567.19	566.72	503.36	501.91
SiH	2041.80	2004.26	2003.60	1984.99	1984.93
SiH^+	2157.20	2099.19	2098.24	2087.80	2087.63
SiF	857.20	834.03	832.48	816.55	814.48
SiCl	535.60	529.88	528.13	516.32	514.51
SiN	1151.40	1189.45	1187.63	1180.29	1177.69
SiO	1241.50	1240.81	1239.82	1216.80	1214.48
SiS	749.60	752.24	751.86	741.85	739.34
P_2	780.80	805.07	806.35	799.29	796.29
P_2^+	672.20	694.91	690.75	697.36	695.51
PH	2365.20	2338.89	2340.47	2301.95	2298.37
PF	846.80	821.18	819.78	805.26	803.52
PCl	551.40	546.05	543.08	530.37	527.60

(continued)

PN	1337.20	1383.85	1383.65	1360.56	1356.78
PO	1233.30	1239.53	1237.23	1208.58	1204.92
S_2	725.60	712.94	707.17	707.40	703.42
SO	1149.20	1133.65	1128.56	1106.03	1102.00
Cl_2	559.70	540.42	539.64	531.01	529.64
Cl_2^+	645.60	630.57	628.79	616.55	614.42
HCl	2990.90	2950.77	2951.14	2919.03	2912.88
HCl^+	2673.70	2611.60	2613.08	2598.43	2594.47
ClF	786.10	762.47	760.95	747.32	745.62
ClO	853.80	851.75	848.58	834.77	831.99
ME		-0.472	-2.301	-20.55	-23.58
MAD		29.99	29.88	36.36	37.72

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 different versions of srTM-L$\tilde{q}$ compared with the experimental values.

Table S4: 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.[S5]

Molecule	Exptl.	srTM-L$\tilde{q}$			
		PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
C	5.50	4.19	4.19	4.15	4.17
Si	1.17	0.68	0.69	0.67	0.67
Ge	0.74	0.40	0.40	0.38	0.35
SiC	2.42	1.50	1.49	1.43	1.42
BN	6.36	4.70	4.71	4.55	4.54
BP	2.10	1.37	1.41	1.34	1.37
AlN	4.90	3.52	3.50	3.41	3.38
AlP	2.50	1.67	1.68	1.68	1.68
AlAs	2.23	1.59	1.61	1.56	1.57
GaN	3.28	1.74	1.72	1.57	1.54
GaP	2.35	1.65	1.65	1.62	1.62
GaAs	1.52	0.90	0.89	0.89	0.86
InP	1.42	0.91	0.90	0.86	0.84
InAs	0.42	0.15	0.15	0.10	0.08
InSb	0.24	0.22	0.21	0.21	0.19
LiH	4.94	3.19	3.18	3.21	3.23
LiF	14.20	9.23	9.23	9.01	9.02
LiCl	9.40	6.56	6.57	6.66	6.67
NaF	11.50	6.19	6.23	6.02	6.03
NaCl	8.50	5.22	5.24	5.26	5.30
MgO	7.83	5.11	5.09	4.87	4.84
ME		-1.56	-1.56	-1.62	-1.63
MAD		1.56	1.56	1.62	1.63

Table S5: Equilibrium lattice constants, a_0 Å comparisons of 55 solids. Experimental values Exptl. are from Ref.,[S6] include zero-point effects.

Molecule	Exptl.	srTM-L$\tilde{q}$			
		PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
C	3.553	3.569	3.572	3.573	3.573
Si	5.421	5.427	5.433	5.437	5.442
Ge	5.644	5.679	5.676	5.709	5.712
Sn	6.477	6.599	6.603	6.602	6.603
SiC	4.346	4.345	4.347	4.361	4.362
BN	3.592	3.604	3.604	3.615	3.618
BP	4.525	4.535	4.538	4.547	4.549
AlN	4.368	4.354	4.356	4.374	4.377
AlP	5.451	5.456	5.459	5.470	5.472
AlAs	5.649	5.655	5.660	5.678	5.681
GaN	4.520	4.547	4.550	4.567	4.570
GaP	5.439	5.493	5.502	5.507	5.513
GaAs	5.640	5.705	5.707	5.717	5.721
InP	5.858	5.947	5.955	5.967	5.973
InAs	6.047	6.142	6.144	6.168	6.170
InSb	6.468	6.587	6.588	6.585	6.595
LiH	3.979	3.960	3.962	3.969	3.972
LiF	3.972	3.969	3.968	3.991	3.996
LiCl	5.070	5.038	5.042	5.046	5.052
NaF	4.582	4.489	4.495	4.510	4.517
NaCl	5.569	5.487	5.493	5.491	5.497
MgO	4.189	4.176	4.178	4.200	4.204
Li	3.443	3.409	3.415	3.399	3.405
Na	4.214	4.121	4.125	4.103	4.106
K	5.212	5.191	5.200	5.182	5.179
Rb	5.577	5.558	5.562	5.548	5.548
Cs	6.039	6.058	6.061	5.991	5.975
Ca	5.556	5.462	5.464	5.470	5.471
Ba	5.002	4.902	4.893	4.922	4.941
Sr	6.040	5.989	5.984	5.962	5.957
Al	4.018	3.984	3.989	3.990	3.993
Fe	2.853	2.807	2.800	2.820	2.810
Co	3.524	3.499	3.498	3.517	3.518
Ni	3.508	3.495	3.495	3.490	3.490
Sc	3.270	3.212	3.212	3.221	3.221
Y	3.594	3.581	3.580	3.579	3.578
Ti	2.915	2.870	2.870	2.876	2.877
Zr	3.198	3.203	3.202	3.221	3.222
Hf	3.151	3.169	3.170	3.162	3.163
V	3.021	2.962	2.962	2.967	2.968
Nb	3.294	3.318	3.319	3.331	3.332
Ta	3.299	3.318	3.319	3.315	3.316
Mo	3.141	3.147	3.148	3.155	3.156
W	3.160	3.179	3.180	3.176	3.176
Tc	2.716	2.722	2.724	2.729	2.730
Re	2.744	2.773	2.774	2.760	2.760
Ru	2.669	2.683	2.684	2.688	2.689
Os	2.699	2.729	2.730	2.723	2.723
Rh	3.794	3.823	3.824	3.822	3.822
Ir	3.831	3.890	3.892	3.879	3.879
Pd	3.876	3.934	3.934	3.927	3.927
Pt	3.913	3.981	3.982	3.974	3.974
Cu	3.595	3.604	3.603	3.592	3.591
Ag	4.062	4.128	4.127	4.115	4.114
Au	4.062	4.165	4.165	4.158	4.158
ME		0.005	0.007	0.009	0.011
MAD		0.040	0.041	0.043	0.044

Table S6: Cohesive energies, $E_{coh}(eV/atom)$ of 55 solids. Experimental values Exptl. are from Ref.,[S6] include zero-point effects.

Molecule	Exptl.	srTM-L$\tilde{q}$			
		PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
C	7.550	7.510	7.480	7.435	7.396
Si	4.680	4.579	4.551	4.548	4.513
Ge	3.890	3.621	3.603	3.668	3.656
Sn	3.160	3.133	3.120	3.215	3.204
SiC	6.480	6.387	6.360	6.317	6.283
BN	6.760	6.860	6.846	6.818	6.799
BP	5.140	5.137	5.097	5.124	5.091
AlN	5.850	5.875	5.861	5.856	5.840
AlP	4.320	4.109	4.074	4.180	4.148
AlAs	3.820	3.725	3.705	3.739	3.715
GaN	4.550	4.465	4.449	4.499	4.486
GaP	3.610	3.444	3.406	3.533	3.503
GaAs	3.340	3.124	3.104	3.168	3.148
InP	3.470	3.103	3.072	3.223	3.197
InAs	3.080	2.861	2.845	2.934	2.916
InSb	2.810	2.548	2.524	2.752	2.742
LiH	2.490	2.473	2.471	2.469	2.467
LiF	4.460	4.475	4.470	4.360	4.352
LiCl	3.590	3.487	3.482	3.466	3.460
NaF	3.970	4.035	4.029	3.923	3.913
NaCl	3.340	3.240	3.233	3.221	3.214
MgO	5.200	5.315	5.305	5.225	5.210
Li	1.670	1.660	1.649	1.652	1.644
Na	1.120	1.109	1.097	1.112	1.102
K	0.940	0.943	0.936	0.942	0.934
Rb	0.860	0.866	0.860	0.869	0.861
Cs	0.810	0.817	0.808	0.821	0.818
Ca	1.870	2.060	2.043	2.039	2.022
Ba	1.910	1.997	1.977	1.988	1.975
Sr	1.730	1.788	1.770	1.793	1.779
Al	3.430	3.559	3.529	3.548	3.525
Fe	4.300	5.243	5.201	5.006	4.977
Co	4.420	5.574	5.313	4.979	4.950
Ni	4.480	4.592	4.745	4.600	4.765
Sc	3.930	4.182	4.173	4.171	4.159
Y	4.390	4.073	4.062	4.131	4.121
Ti	4.880	5.331	5.337	5.265	5.249
Zr	6.270	5.194	5.221	5.415	5.432
Hf	6.460	6.284	6.275	6.449	6.443
V	5.350	5.536	5.546	6.333	5.588
Nb	7.600	6.774	6.795	7.002	7.021
Ta	8.130	7.983	7.988	8.244	8.248
Mo	6.860	6.513	6.568	6.686	6.721
W	8.940	8.181	8.194	8.524	8.538
Tc	6.880	6.966	7.043	7.072	7.105
Re	8.050	7.627	7.684	7.893	7.931
Ru	6.770	6.772	6.801	6.717	6.707
Os	8.200	7.879	7.903	8.207	8.232
Rh	5.780	5.559	5.568	5.599	5.596
Ir	6.990	6.712	7.006	7.062	7.090
Pd	3.930	4.026	4.046	4.178	4.193
Pt	5.870	5.241	5.244	5.566	5.559
Cu	3.510	3.821	3.833	3.934	3.939
Ag	2.960	2.861	2.864	2.935	2.935
Au	3.830	3.279	3.278	3.334	3.330
ME		-0.076	-0.077	-0.017	-0.035
MAD		0.236	0.232	0.186	0.179

Table S7: Bulk modulus, $B_0(GPa)$ of 44 cubic solids. Experimental values Exptl. are from Ref.,[S7] these values were obtained by subtracting the zero-point phonon effect from the experimental zero-temperature values.

Molecule	Exptl.	srTM-L$\tilde{q}$			
		PC_{rep}		PC_{opt}	
		Scheme 1	Scheme 2	Scheme 1	Scheme 2
C	454.700	431.411	432.727	429.391	428.167
Si	101.300	93.701	92.736	90.694	90.428
Ge	79.400	74.869	74.677	72.356	72.286
Sn	42.800	38.008	38.158	36.947	36.886
SiC	229.100	216.448	218.071	216.529	215.635
BN	410.200	382.433	383.255	378.527	372.560
BP	168.000	168.971	167.289	160.784	158.870
AlN	206.000	213.650	212.935	201.919	200.508
AlP	87.400	92.463	90.380	89.567	88.788
AlAs	75.000	76.323	75.235	73.623	73.382
GaN	213.000	199.969	199.197	191.613	190.282
GaP	89.600	86.818	85.281	88.982	87.207
GaAs	76.700	68.746	68.716	71.551	70.655
InP	72.000	73.097	69.097	70.160	69.443
InAs	58.600	56.556	55.885	52.381	51.383
InSb	46.100	46.276	46.307	46.031	43.358
LiH	40.100	41.009	40.760	39.831	39.781
LiF	76.300	85.255	81.736	82.162	82.274
LiCl	38.700	40.764	40.689	39.459	39.413
NaF	53.100	65.199	63.270	56.822	56.362
NaCl	27.600	32.909	32.366	33.013	32.825
MgO	169.800	176.239	175.302	166.448	165.495
Li	13.100	14.549	14.854	14.664	14.413
Na	7.900	8.487	6.738	8.696	8.847
K	3.800	4.242	4.259	4.015	3.706
Rb	3.600	3.245	3.278	3.544	3.185
Cs	2.300	2.278	2.281	2.533	2.884
Ca	15.900	19.149	19.420	18.946	19.018
Ba	10.600	10.914	11.234	9.537	8.522
Sr	12.000	11.874	11.725	11.541	11.491
Al	77.100	88.329	87.535	86.653	86.259
Ni	192.500	212.376	213.322	216.786	216.977
V	165.800	196.582	196.940	199.635	199.571
Nb	173.200	177.355	177.491	177.091	177.325
Ta	202.700	203.663	204.510	208.550	209.017
Mo	276.200	272.322	272.761	273.254	273.148
W	327.500	318.247	318.669	318.950	319.082
Rh	277.100	261.101	261.909	268.384	268.728
Ir	362.200	341.222	341.598	346.316	346.398
Pd	187.200	174.143	175.104	180.243	180.909
Pt	285.500	248.078	248.855	250.533	250.664
Cu	144.300	144.499	145.990	154.780	155.446
Ag	105.700	98.319	98.885	102.460	102.929
Au	182.000	140.740	141.103	143.483	143.737
ME		-2.974	-3.208	-3.507	-3.988
MAD		8.670	8.455	8.583	9.057

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 S8: 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
*sr*TM	-0.6751	2.17
*sr*TM-L (PC_{rep})	-0.6880	2.15
*sr*TM-L$\tilde{q}$ (PC_{opt})	-0.7250	2.12

Table S9: As in Table S8 for fcc Co.

XC functional	Energy eV	Magnetization μ_B
Exp.		1.72
PBE	-0.2055	1.64
*sr*TM-L$\tilde{q}$ (PC_{opt})	-0.2621	1.77
*sr*TM	-0.2946	1.73
*sr*TM-L(PC_{rep})	-0.3045	1.75

Table S10: As in Table S8 for fcc Ni.

XC functional	Energy eV	Magnetization μ_B
Exp.		0.62
PBE	-0.0583	0.63
*sr*TM	-0.0814	0.66
*sr*TM-L(PC_{rep})	-0.0856	0.69
*sr*TM-L$\tilde{q}$ (PC_{opt})	-0.1069	0.75

Table S11: As in Table S8 for hcp Co.

XC functional	Energy eV	Magnetization μ_B
Exp.		1.57
PBE	-0.2369	1.60
*sr*TM	-0.2808	1.61
*sr*TM-L(PC_{rep})	-0.3107	1.65
*sr*TM-L$\tilde{q}$ (PC_{opt})	-0.3302	1.60

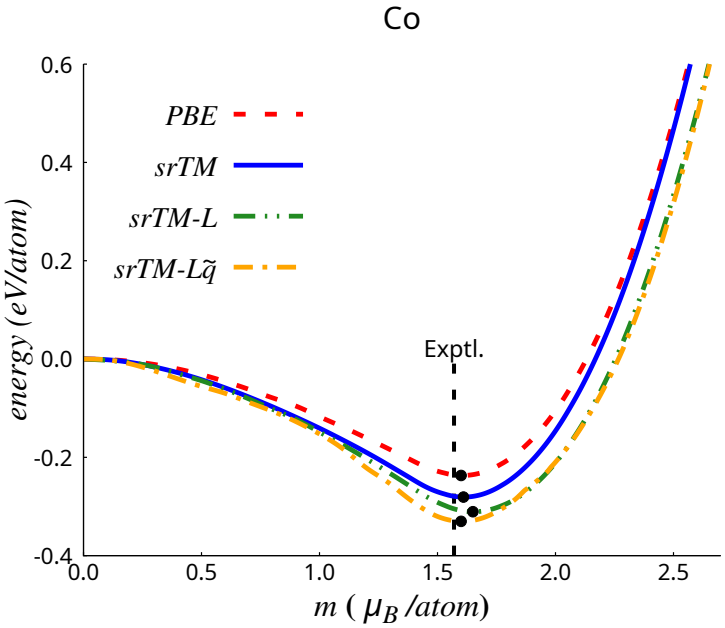

Figure S1: Fixed spin moment energy for hcp Co using calculated equilibrium latticce parameter, on a per-atom basis for. Comparation of different functionals.

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