Supplemental Information
Performance Improvement of De-orbitalized Exchange-Correlation Functionals

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(Dated: 21 January 2026; version 5 revised, minor edits)

We provide a detailed, system-by-system tabulation of the numerical results from the tests against standard molecular and crystalline system datasets reported in the main paper. Additionally, we present the timing and SCF cycle data for each system. Plots of mean-squared displacement and radial distribution functions for AIMD calculations on Al also are provided as are XC energies for light atoms from different deorbitalizers.

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I. MOLECULAR TEST SET RESULTS CALCULATED IN NWCHEM-7.0.2

Here we provide the molecule-by-molecule tabulation for the G3X/99, T96R, and T82-F test sets for r^{2}SCAN-L(SRPP) and r^{2}SCAN-L(SRPP2) compared r^{2}SCAN-L(RPP), r^{2}SCAN-L(PC$_{opt}$), r^{2}SCAN, and PBE. Calculations were performed in NWChem-7.0.2.

TABLE I: Standard enthalpies of formation (ΔH_f) in kcal/mol for the G3X/99 molecular test set [1, 2] obtained with different approximate exchange-correlation functionals.

Molecule	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC$_{opt}$	RPP	SRPP	SRPP2
LiH	33.30	38.353	36.369	37.109	38.488	38.881	38.795
^{2}BeH	81.70	77.032	72.401	71.715	74.162	75.041	74.646
^{2}CH	142.50	141.870	145.246	142.898	144.376	144.171	143.904
CH_2 ($^3B_1$)	93.60	89.512	87.380	89.023	94.579	91.488	90.633
CH_2 ($^1A_1$)	102.60	104.969	109.080	107.423	110.890	109.342	108.542
$^3CH_3$	35.00	32.400	31.093	33.253	39.942	36.104	34.880
CH_4	-17.80	-18.051	-16.985	-13.443	-7.328	-12.772	-14.220
^{3}NH	85.80	80.598	84.819	80.954	82.511	82.919	82.571
NH_2 ($^2B_1$)	44.50	38.882	43.940	39.917	43.451	42.895	41.889
NH_3	-10.90	-14.099	-6.591	-9.316	-4.542	-7.733	-9.205
^{2}OH	9.00	6.631	7.906	6.770	9.753	8.647	7.724
H_2O	-57.80	-58.172	-54.083	-53.778	-49.566	-53.726	-55.183
HF	-65.20	-65.067	-61.578	-59.851	-58.837	-62.209	-62.758
SiH_2 ($^1A_1$)	65.20	68.485	67.659	68.505	69.003	67.418	67.196
SiH_2 ($^3B_1$)	86.20	84.892	78.683	80.106	82.052	80.344	80.042
$^2SiH_3$	47.90	50.421	43.307	45.945	47.712	45.649	45.320
SiH_4	8.20	16.150	8.051	12.501	13.952	11.518	11.153
$^2PH_2$	33.10	31.274	30.299	30.770	29.155	28.182	27.899
PH_3	1.30	3.543	2.916	4.561	2.439	0.385	-0.088
H_2S	-4.90	-4.615	-4.802	-2.944	-3.270	-5.743	-6.386
HCl	-22.00	-21.934	-21.697	-20.269	-20.172	-22.148	-22.550
Li_2	51.60	56.191	57.947	57.313	57.488	57.661	57.655
LiF	-80.10	-79.231	-75.223	-72.315	-69.395	-71.367	-71.827
HC≡CH	54.60	45.137	57.291	58.892	70.731	61.509	59.282
$H_2C{=}CH_2$	12.50	4.228	13.271	16.661	26.686	17.066	14.668
$H_3C{-}CH_3$	-20.10	-25.214	-19.899	-14.284	-5.363	-15.728	-18.362
CN	105.20	89.042	108.285	101.621	106.756	103.364	101.808
HCN	30.90	18.183	36.347	32.404	40.459	34.832	32.933
CO	-26.40	-36.038	-22.494	-22.436	-18.136	-23.539	-25.127
^{2}HCO	10.00	-6.433	6.377	5.781	10.996	4.729	2.848
H_2CO	-26.10	-38.135	-25.490	-24.880	-19.393	-26.569	-28.626
CH_3OH	-48.00	-55.038	-46.549	-44.067	-38.712	-47.105	-49.562
N_2	0.00	-14.907	8.712	-0.240	3.665	1.488	-0.069
H_2NNH_2	23.30	12.788	32.413	24.446	28.848	23.506	21.009
NO	21.80	2.200	22.182	15.018	15.838	13.142	11.602
$^3O_2$	0.00	-23.578	-9.495	-12.965	-13.200	-17.465	-19.152
H_2O_2	-32.40	-45.264	-31.281	-35.353	-33.654	-39.707	-41.969
F_2	0.00	-14.480	-0.542	-4.667	-9.508	-13.249	-13.597
CO_2	-94.00	-121.233	-99.730	-97.447	-89.673	-101.003	-103.914
Na_2	34.00	33.232	37.360	37.546	37.309	36.854	36.872
Si_2	139.90	133.292	140.050	135.912	135.809	133.390	132.993
P_2	34.30	29.927	38.906	36.922	31.634	29.689	29.260

(continued)

$^3S_2$	30.70	17.177	21.557	22.318	19.389	17.009	16.410
Cl_2	0.00	-7.570	-1.173	-1.638	-6.232	-8.116	-8.412
NaCl	-43.60	-39.225	-42.209	-39.092	-36.391	-38.507	-38.810
SiO	-24.60	-27.933	-19.627	-19.149	-17.709	-21.460	-22.626
CS	66.90	58.405	69.398	68.214	69.111	65.195	64.242
SO	1.20	-14.255	-5.788	-6.158	-7.464	-10.376	-11.520
ClO	24.30	7.982	18.816	15.974	12.640	10.749	9.866
ClF	-13.30	-23.623	-13.513	-14.553	-19.598	-22.196	-22.508
Si_2H_6	19.10	28.424	16.115	23.590	25.329	20.106	19.281
CH_3Cl	-19.60	-25.231	-20.538	-17.375	-15.031	-21.253	-22.731
H_3C-SH	-5.50	-10.501	-6.357	-2.615	-0.062	-7.194	-8.996
HOCl	-18.40	-28.359	-18.260	-20.219	-21.552	-25.619	-26.908
SO_2	-71.00	-91.183	-72.660	-71.378	-74.596	-80.887	-83.080
BF_3	-271.40	-282.638	-273.732	-261.174	-256.651	-269.966	-271.941
BCl_3	-96.30	-110.171	-106.297	-100.432	-98.153	-107.472	-109.273
AlF_3	-289.00	-287.468	-286.282	-273.842	-269.090	-278.243	-279.569
$AlCl_3$	-139.70	-140.648	-147.936	-138.944	-135.898	-143.382	-144.598
CF_4	-223.10	-250.932	-229.516	-216.625	-224.583	-241.665	-243.667
CCl_4	-22.90	-44.635	-29.324	-27.076	-35.948	-46.195	-47.887
OCS	-33.10	-59.555	-42.142	-40.244	-36.043	-45.558	-47.829
CS_2	28.00	3.687	16.922	18.742	19.700	11.663	10.017
F_2CO	-145.00	-174.364	-151.353	-144.425	-144.906	-159.009	-161.468
SiF_4	-386.00	-383.670	-381.350	-362.250	-363.452	-376.778	-378.308
$SiCl_4$	-158.40	-162.572	-165.540	-154.410	-158.553	-168.382	-169.721
NNO	19.70	-20.819	14.882	5.088	7.926	0.951	-1.727
ClNO	12.60	-21.066	5.366	-3.159	-5.385	-10.076	-11.896
NF_3	-31.60	-71.956	-40.578	-45.794	-58.061	-65.961	-67.282
PF_3	-229.10	-239.427	-226.170	-216.140	-225.884	-234.636	-235.573
O_3	33.90	-3.619	29.247	18.630	14.112	7.478	4.885
F_2O	5.90	-24.698	-1.016	-7.977	-16.486	-21.895	-23.017
ClF_3	-38.00	-76.974	-52.045	-52.659	-66.611	-73.859	-74.605
$F_2C=CF_2$	-161.30	-204.597	-170.535	-160.217	-164.578	-185.773	-188.788
$Cl_2C=CCl_2$	-5.50	-38.126	-14.830	-10.984	-15.617	-31.073	-33.806
F_3C-CN	-118.40	-160.508	-121.756	-117.287	-116.562	-136.050	-139.571
$HC\equiv C-CH_3$	44.40	28.038	44.560	49.244	63.940	49.342	45.899
$H_2C=C=CH_2$	45.40	24.612	41.757	46.143	60.601	45.917	42.467
C_3H_4 (cyclopropene)	67.80	47.295	65.517	69.956	82.220	67.607	64.169
$H_2C=CH-CH_3$	4.80	-8.811	4.184	10.216	23.177	8.315	4.682
C_3H_6 (cyclopropane)	12.80	-2.957	10.333	17.650	28.768	13.556	9.884
$CH_3-CH_2-CH_3$	-25.10	-34.289	-25.256	-17.376	-5.608	-20.978	-24.826
C_4H_6 (Z-1,3-butadiene)	26.40	3.800	24.253	30.580	47.777	28.493	23.875
C_4H_6 (2-butyne)	34.80	12.610	33.601	41.191	58.692	38.759	34.113
C_4H_6 (methylenecyclopropane)	47.90	19.512	41.192	49.145	64.307	44.355	39.677
C_4H_6 (bicyclo[1.1.0]butane)	51.90	26.702	48.326	57.165	69.721	49.869	45.194
C_4H_6 (cyclobutene)	38.20	14.490	36.791	43.603	57.046	37.621	33.007
C_4H_8 (cyclobutane)	6.60	-12.675	5.204	13.579	26.156	6.250	1.429
C_4H_8 (isobutene)	-4.10	-21.712	-5.292	3.326	19.254	-0.839	-5.716
C_4H_{10} (trans butane)	-30.10	-43.284	-30.572	-20.449	-5.786	-26.178	-31.241
C_4H_{10} (isobutane)	-32.20	-44.374	-32.187	-21.989	-7.333	-27.770	-32.855
C_5H_8 (spiropentane)	44.30	11.935	37.527	49.222	65.188	39.936	34.018
C_6H_6 (benzene)	19.90	-22.848	10.403	21.101	42.493	13.496	6.888
CH_2F_2	-107.70	-122.140	-109.028	-102.636	-104.588	-114.499	-116.089

(continued)

CHF_3	-166.30	-187.903	-170.262	-160.693	-165.861	-179.191	-180.972
CH_2Cl_2	-22.60	-33.914	-25.527	-22.453	-23.821	-31.216	-32.759
$CHCl_3$	-24.50	-41.183	-29.246	-26.387	-31.446	-40.244	-41.865
CH_3NH_2	-5.20	-5.273	5.683	4.732	12.571	5.121	2.599
CH_3CN	18.00	-2.068	20.217	19.696	30.763	19.744	16.613
CH_3NO_2 (nitromethane)	-17.90	-59.555	-25.879	-29.863	-27.474	-40.374	-44.455
CH_3ONO (methyl nitrite)	-16.10	-54.847	-21.287	-27.059	-26.280	-37.794	-41.678
CH_3SiH_3	-7.00	-2.305	-7.007	0.193	6.147	-1.682	-3.444
HCO_2H	-90.40	-111.954	-93.046	-90.478	-84.584	-96.346	-99.582
HCO_2CH_3	-85.50	-111.885	-89.540	-84.805	-77.811	-93.556	-97.816
CH_3CONH_2	-57.00	-84.231	-58.876	-56.622	-45.506	-62.058	-66.701
C_2H_5N (aziridine)	30.20	10.031	30.296	31.194	38.577	26.678	23.229
NCCN (cyanogen)	74.10	37.081	77.596	68.762	82.690	71.074	67.493
$NH(CH_3)_2$	-4.30	-17.806	-1.721	-0.130	8.350	-4.200	-7.877
$CH_3CH_2NH_2$	-11.30	-25.203	-9.440	-7.713	1.895	-11.031	-14.814
$H_2C{=}C{=}O$ (ketene)	-11.60	-37.267	-17.674	-14.523	-3.535	-16.487	-19.708
C_2H_4O (oxirane)	-12.60	-32.026	-15.115	-11.040	-5.591	-17.633	-20.918
CH_3CHO	-39.50	-57.475	-41.209	-37.277	-28.472	-41.076	-44.422
$O{=}CH{-}CH{=}O$	-50.80	-80.457	-52.935	-51.983	-43.124	-57.648	-61.646
CH_3CH_2OH	-56.10	-67.563	-55.501	-50.440	-42.006	-55.565	-59.256
$(CH_3)_2O$	-44.00	-56.457	-44.134	-39.194	-32.769	-45.451	-48.955
C_2H_4S (thiooxirane)	19.60	2.869	15.131	20.141	23.976	12.743	10.001
$(CH_3)_2S{=}O$	-36.20	-55.337	-40.593	-33.373	-29.153	-43.819	-47.823
CH_3CH_2SH	-11.10	-19.965	-12.118	-6.069	-0.674	-12.826	-15.841
$(CH_3)_2S$	-8.90	-19.041	-10.926	-4.989	0.351	-11.534	-14.524
$H_2C{=}CHF$	-34.00	-51.223	-35.880	-30.799	-24.387	-36.715	-39.272
CH_3CH_2Cl	-26.60	-36.728	-28.392	-22.771	-17.486	-28.803	-31.503
$H_2C{=}CHCl$	5.20	-9.818	2.760	6.443	13.055	1.981	-0.521
$H_2C{=}CHCN$	43.20	15.936	46.042	45.318	60.734	45.347	41.245
$(CH_3)_2C{=}O$	-51.70	-73.961	-54.629	-47.703	-35.595	-53.515	-58.134
CH_3CO_2H	-103.40	-128.749	-106.948	-101.283	-92.016	-109.083	-113.591
CH_3CFO	-105.70	-131.162	-109.997	-102.930	-97.143	-113.010	-116.537
CH_3COCl	-57.70	-83.546	-64.631	-59.903	-53.932	-68.269	-71.741
$CH_3CH_2CH_2Cl$	-31.50	-45.698	-33.686	-25.818	-17.623	-33.961	-37.875
$(CH_3)_2CHOH$	-65.20	-80.323	-65.178	-57.559	-46.077	-64.818	-69.763
$CH_3{-}O{-}CH_2CH_3$	-51.70	-68.837	-52.970	-45.482	-35.953	-53.800	-58.539
$(CH_3)_3N$	-6.60	-23.659	-4.148	-0.171	10.043	-7.215	-12.042
C_4H_4O (furan)	-8.30	-46.264	-15.438	-8.334	4.237	-18.338	-23.736
C_4H_4S (thiophene)	27.50	-6.991	18.924	27.078	37.979	16.520	11.710
C_4H_5N (pyrrole)	25.90	-13.692	20.536	25.053	40.075	17.299	11.688
C_5H_5N (pyridine)	33.60	-14.365	25.893	30.671	48.297	22.474	16.126
H_2	0.00	4.886	2.029	3.370	3.410	3.368	3.417
^2SH	34.20	33.105	32.445	33.084	32.995	32.098	31.762
$^2C{\equiv}CH$	135.80	123.889	134.490	134.664	144.771	137.445	135.527
'$HC{=}CH_2$ ($^2A''$)'	71.00	58.415	66.139	68.536	78.514	70.159	67.945
'$CH_3C{=}O$ ($^2A''$)'	-2.40	-24.710	-8.016	-5.418	3.101	-8.303	-11.457
$CH_2{-}OH$ (^2A)	-4.00	-15.885	-7.899	-6.516	-0.494	-8.124	-10.454
'CH_3O ($^2A''$)'	5.20	-8.513	-1.003	0.761	4.779	-1.301	-3.349
'CH_3CH_2O ($^2A''''$)'	-2.90	-22.343	-10.758	-6.431	0.716	-10.633	-13.938
'CH_3S ($^2A''$)'	29.80	21.234	25.434	28.251	30.912	25.097	23.561
'CH_2CH_3 ($^2A''$)'	28.60	19.913	23.478	28.166	37.670	28.561	26.099
'$(CH_3)_2CH$ ($^2A''$)'	21.10	6.724	14.611	21.949	34.258	19.887	16.179

(continued)

$^2C(CH_3)_3$	12.00	-6.483	5.238	15.230	30.353	10.727	5.769
NO_2 ($^2A_1$)	8.10	-34.634	-3.219	-11.088	-10.985	-18.254	-20.937
$CH_3CH{=}C{=}CH_2$	38.80	13.314	34.599	41.379	58.641	38.879	34.225
C_5H_8 (isoprene)	18.00	-8.185	15.537	24.329	44.500	19.955	14.087
C_5H_{10} (cyclopentane twist)	-18.50	-40.154	-20.086	-8.784	6.056	-18.992	-25.018
C_5H_{12} (n-pentane)	-35.00	-52.206	-35.811	-23.446	-5.903	-31.313	-37.590
$C(CH_3)_4$ (neopentane)	-40.10	-54.531	-39.783	-27.331	-9.772	-35.302	-41.633
C_6H_8 (1,3-cyclohexadiene)	25.40	-9.671	21.575	32.086	52.102	22.770	15.938
C_6H_8 (1,4-cyclohexadiene)	25.00	-9.517	21.779	32.585	52.561	23.099	16.269
C_6H_{12} (cyclohexane chair)	-29.40	-53.494	-30.893	-17.059	0.430	-29.727	-36.979
C_6H_{14} (n-hexane)	-39.90	-61.144	-41.090	-26.405	-6.035	-36.466	-43.957
C_6H_{14} (3-methylpentane)	-41.10	-60.442	-41.004	-26.565	-5.986	-36.574	-44.105
$C_6H_5{-}CH_3$ (toluene)	12.00	-34.726	2.192	15.416	39.784	5.516	-2.334
C_7H_{16} (n-heptane)	-44.80	-70.074	-46.317	-29.454	-6.159	-41.607	-50.311
C_8H_8 (cyclooctatetraene)	70.70	18.532	65.076	76.464	104.517	66.069	57.259
C_8H_{18} (n-octane)	-49.80	-79.015	-51.578	-32.464	-6.294	-46.761	-56.679
$C_{10}H_8$ (naphtalene)	35.90	-40.015	17.424	34.814	67.806	19.324	8.479
$C_{10}H_8$ (azulene)	69.10	-9.667	50.165	66.252	98.858	50.559	39.732
$CH_3CO_2CH_3$ (Z-methylacetate)	-98.40	-128.162	-102.893	-95.109	-84.780	-105.839	-111.368
$(CH_3)_3COH$ (t-butanol)	-74.70	-92.259	-74.627	-64.578	-50.031	-73.939	-80.139
$C_6H_5NH_2$ (aniline)	20.80	-32.284	11.151	18.846	41.803	9.289	1.429
C_6H_5OH (phenol)	-22.30	-73.497	-33.497	-22.547	-1.046	-34.143	-41.898
C_4H_6O (divinyl ether)	-3.30	-35.231	-7.406	-0.764	15.040	-7.723	-13.362
C_4H_8O (tetrahydrofuran)	-44.00	-68.725	-45.741	-36.685	-26.990	-49.454	-55.151
C_5H_8O (cyclopentanone)	-45.90	-81.653	-51.377	-40.705	-25.457	-53.185	-59.983
$C_6H_4O_2$ (benzoquinone)	-29.40	-90.551	-38.774	-31.421	-10.476	-44.335	-52.596
$C_6H_4N_2$ (pyrimidine)	46.80	-7.724	39.251	38.453	52.198	29.572	23.490
$(CH_3)_2SO_2$	-89.20	-113.367	-95.574	-83.642	-79.846	-98.481	-103.578
C_6H_5Cl (chlorobenzene)	12.50	-36.164	0.253	11.245	29.304	-1.241	-7.953
$NC(CH_2)_2CN$ (succinonitrile)	50.10	7.507	54.670	51.985	71.011	49.465	43.443
$C_4H_4N_2$ (pyrazine)	46.90	-4.086	43.407	42.011	55.803	33.188	27.104
C_4H_4O (3-butyn-2-one)	15.60	-15.729	15.244	20.204	38.382	16.376	10.992
C_4H_6O (E-crotonaldehyde)	-24.00	-57.070	-29.433	-22.649	-6.729	-28.937	-34.487
$C_4H_6O_3$ (acetic anhydride)	-136.80	-185.596	-146.708	-136.689	-122.482	-151.813	-159.349
C_4H_6S (2,5-dihydrothiophene)	20.80	-7.106	15.945	23.923	33.493	12.266	7.312
$(CH_3)_2CHCN$	5.60	-20.146	9.229	13.050	29.878	8.953	3.403
C_4H_8O (methyl ethyl ketone)	-57.10	-83.160	-60.325	-51.134	-36.094	-59.137	-64.965
$(CH_3)_2CHCHO$	-51.60	-75.639	-52.368	-43.945	-29.397	-52.021	-57.797
$C_4H_8O_2$ (1,4-dioxane)	-75.50	-107.583	-78.669	-69.832	-62.338	-87.509	-94.135
C_4H_8S (tetrahydrothiophene)	-8.20	-29.721	-10.968	-1.369	6.905	-14.680	-19.842
$(CH_3)_3CCl$	-43.50	-59.576	-45.684	-35.297	-24.120	-45.685	-50.868
C_4H_9Cl (n-butyl chloride)	-37.00	-54.560	-38.869	-28.722	-17.684	-39.037	-44.162
C_4H_9N (tetrahydropyrrole)	-0.80	-27.032	-0.164	5.179	16.786	-5.429	-11.295
$C_4H_9NO_2$ (2-nitrobutane)	-39.10	-90.951	-47.460	-44.384	-33.132	-61.343	-69.092
$(CH_3CH_2)_2O$	-60.30	-81.093	-61.704	-51.628	-39.040	-62.043	-68.016
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	-93.10	-119.944	-95.091	-85.050	-74.404	-100.258	-107.147
$(CH_3)_3CSH$	-26.20	-41.107	-27.472	-16.801	-5.750	-28.079	-33.571
$C_4H_{10}S_2$ (diethyl disulfide)	-17.90	-41.111	-22.447	-11.194	-3.600	-27.206	-32.958
$(CH_3)_3CNH_2$	-28.90	-47.647	-26.378	-19.879	-4.314	-27.480	-33.760
$(CH_3)_4Si$	-55.70	-58.530	-54.175	-38.488	-19.037	-43.230	-49.208
C_5H_6S (2-methyl thiophene)	20.00	-18.880	10.745	21.461	35.233	8.583	2.554
C_5H_7N (N-methyl pyrrole)	24.60	-19.073	18.955	25.792	42.655	15.208	8.486

(continued)

$C_5H_{10}O$ (tetrahydropyran)	-53.40	-81.279	-55.557	-44.128	-31.617	-59.313	-66.256
$(CH_3CH_2)_2C{=}O$	-61.60	-92.252	-65.921	-54.472	-36.522	-64.663	-71.699
$C_5H_{10}O_2$ (isopropyl acetate)	-115.10	-152.246	-120.534	-107.716	-91.176	-122.609	-130.627
$C_5H_{10}S$ (tetrahydrothiopyran)	-15.20	-40.167	-18.399	-6.440	4.568	-22.158	-28.558
$C_5H_{11}N$ (piperidine)	-11.30	-39.964	-10.425	-2.564	11.789	-15.637	-22.740
$C_5H_{12}O$ (t-butyl methyl ether)	-67.80	-89.665	-68.525	-56.363	-40.583	-68.810	-76.062
$C_6H_4F_2$ (1,3-difluorobenzene)	-73.90	-133.695	-88.648	-74.292	-59.581	-94.401	-101.351
$C_6H_4F_2$ (1,4-difluorobenzene)	-73.30	-132.983	-87.757	-73.541	-58.821	-93.618	-100.565
C_6H_5F (fluorobenzene)	-27.40	-78.603	-39.430	-26.907	-8.868	-40.758	-47.536
$C_6H_{14}O$ (diisopropyl ether)	-76.30	-103.079	-77.839	-62.933	-44.053	-77.412	-85.894
PF_5	-381.10	-391.911	-380.254	-360.011	-373.306	-389.618	-391.304
SF_6	-291.70	-323.703	-303.621	-284.615	-306.738	-326.133	-328.112
P_4	14.10	-6.429	9.944	11.530	-5.602	-11.092	-12.103
SO_3	-94.60	-125.370	-102.558	-98.006	-100.646	-111.560	-114.877
SCl_2	-4.20	-18.677	-9.243	-8.592	-16.660	-20.143	-20.774
$POCl_3$	-133.80	-151.623	-140.862	-133.935	-142.633	-152.308	-154.255
PCl_5	-86.10	-108.417	-99.199	-93.756	-109.160	-119.035	-120.407
Cl_2O_2S	-84.80	-116.410	-96.999	-91.340	-100.218	-111.235	-113.998
PCl_3	-69.00	-83.704	-74.777	-71.565	-81.537	-87.130	-87.959
Cl_2S_2	-4.00	-31.124	-18.120	-16.570	-27.878	-33.229	-34.239
$SiCl_2$ ($^1A_1$)	-40.30	-46.440	-42.734	-38.579	-41.576	-46.382	-47.064
CF_3Cl	-169.70	-197.941	-177.683	-167.722	-175.898	-191.229	-193.154
C_2F_6	-320.90	-367.896	-332.636	-313.857	-326.062	-353.577	-357.042
$^2CF_3$	-111.80	-139.910	-122.127	-113.933	-118.495	-131.068	-132.697
$^2C_6H_5$ (phenyl radical)	80.50	33.117	65.334	74.912	96.156	68.558	62.136
ME		-20.878	-3.145	1.845	8.796	-5.918	-9.470
MAD		21.385	4.488	5.300	13.109	7.804	10.405
Spread		88.091	29.818	42.938	72.117	48.329	46.036

TABLE II: Bond lengths in $\AA$ for the T96-R molecular test set [3, 4] from different approximate XC functionals.

Molecule	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC$_{opt}$	RPP	SRPP	SRPP2
H_2	0.741	0.751	0.742	0.742	0.747	0.752	0.752
Li_2	2.673	2.738	2.762	2.729	2.727	2.722	2.746
LiH	1.595	1.607	1.605	1.595	1.6	1.608	1.609
LiF	1.564	1.576	1.574	1.569	1.575	1.574	1.573
LiCl	2.021	2.021	2.029	2.016	2.025	2.021	2.021
LiO	1.688	1.699	1.696	1.691	1.701	1.698	1.698
Be_2	2.440	2.441	2.489	2.395	2.439	2.453	2.441
BeH	1.343	1.362	1.357	1.349	1.354	1.364	1.365
BeF	1.361	1.382	1.374	1.373	1.378	1.38	1.379
BeO	1.331	1.346	1.335	1.336	1.345	1.332	1.345
BeS	1.742	1.759	1.749	1.744	1.753	1.746	1.755
B_2	1.590	1.619	1.618	1.609	1.631	1.616	1.625
BH	1.232	1.252	1.242	1.240	1.251	1.257	1.258
BF	1.263	1.276	1.267	1.270	1.277	1.277	1.276
BF_3	1.313	1.325	1.314	1.318	1.321	1.321	1.321
BCl	1.715	1.732	1.724	1.722	1.738	1.734	1.733
BCl_3	1.742	1.748	1.742	1.740	1.745	1.743	1.743
BN	1.281	1.333	1.321	1.323	1.336	1.335	1.333
BO	1.204	1.215	1.206	1.209	1.217	1.216	1.216
BS	1.609	1.621	1.612	1.610	1.621	1.611	1.619
C_2	1.242	1.404	1.249	1.394	1.411	1.25	1.406
CH	1.120	1.137	1.126	1.125	1.138	1.14	1.140
CH_4	1.087	1.096	1.088	1.088	1.096	1.097	1.098
CF	1.272	1.287	1.278	1.285	1.293	1.288	1.287
CF_4	1.323	1.337	1.325	1.333	1.335	1.333	1.333
CCl	1.645	1.660	1.654	1.657	1.67	1.664	1.662
CCl_4	1.767	1.782	1.774	1.778	1.777	1.775	1.775
CN	1.172	1.174	1.165	1.169	1.179	1.177	1.176
CO	1.128	1.136	1.127	1.132	1.139	1.138	1.137
CO^+	1.115	1.122	1.112	1.116	1.125	1.123	1.123
CO_2	1.160	1.171	1.162	1.167	1.173	1.172	1.172
CP	1.562	1.567	1.555	1.556	1.566	1.564	1.563
CS	1.535	1.546	1.536	1.539	1.549	1.546	1.545
CS_2	1.553	1.562	1.553	1.554	1.561	1.559	1.559
N_2	1.098	1.103	1.093	1.099	1.105	1.104	1.104
N_2^+	1.116	1.114	1.106	1.110	1.119	1.116	1.116
NH	1.036	1.051	1.041	1.043	1.052	1.054	1.054
NH^+	1.070	1.091	1.078	1.080	1.087	1.091	1.091
NF	1.317	1.327	1.319	1.330	1.335	1.329	1.328
NCl	1.611	1.618	1.616	1.622	1.629	1.624	1.622
NO	1.151	1.158	1.148	1.155	1.162	1.159	1.158
NO^+	1.063	1.070	1.059	1.066	1.072	1.071	1.070
NS	1.494	1.506	1.494	1.500	1.507	1.505	1.505
O_2	1.208	1.219	1.207	1.218	1.224	1.219	1.219
O_2^+	1.116	1.122	1.109	1.119	1.126	1.122	1.122
OH	0.970	0.983	0.973	0.975	0.985	0.985	0.984
OH^+	1.029	1.048	1.035	1.038	1.042	1.046	1.046
OF	1.358	1.360	1.350	1.364	1.361	1.356	1.355
F_2	1.412	1.413	1.399	1.415	1.407	1.403	1.403

(continued)

F_2^+	1.322	1.316	1.298	1.318	1.312	1.309	1.309
HF	0.917	0.930	0.921	0.924	0.931	0.931	0.931
HF^+	1.001	1.023	1.010	1.011	1.017	1.017	1.018
Na_2	3.079	3.079	3.142	3.120	3.079	3.111	3.113
NaH	1.887	1.893	1.898	1.887	1.887	1.892	1.893
NaF	1.926	1.940	1.926	1.926	1.932	1.923	1.923
NaCl	2.361	2.367	2.365	2.357	2.356	2.351	2.351
NaO	2.052	2.070	2.056	2.053	2.06	2.052	2.052
MgH	1.730	1.757	1.745	1.735	1.742	1.747	1.748
MgF	1.750	1.784	1.766	1.766	1.76	1.766	1.766
MgCl	2.196	2.226	2.212	2.204	2.203	2.196	2.205
MgO	1.748	1.750	1.736	1.737	1.739	1.739	1.739
Al_2	2.466	2.488	2.471	2.462	2.476	2.47	2.470
AlH	1.648	1.679	1.661	1.656	1.661	1.667	1.668
AlF	1.654	1.684	1.664	1.666	1.667	1.668	1.667
AlCl	2.130	2.163	2.145	2.140	2.142	2.143	2.142
AlO	1.618	1.633	1.619	1.619	1.627	1.624	1.624
AlS	2.029	2.049	2.031	2.028	2.035	2.035	2.034
Si_2	2.246	2.287	2.152	2.263	2.269	2.269	2.269
SiH	1.520	1.545	1.530	1.524	1.532	1.537	1.537
SiH_4	1.480	1.493	1.482	1.479	1.484	1.489	1.489
SiF	1.601	1.632	1.613	1.617	1.618	1.618	1.618
SiF_4	1.553	1.580	1.564	1.567	1.569	1.569	1.569
SiCl	2.058	2.084	2.070	2.067	2.072	2.068	2.068
$SiCl_4$	2.019	2.039	2.025	2.024	2.027	2.025	2.025
SiN	1.572	1.580	1.569	1.570	1.576	1.575	1.575
SiO	1.510	1.529	1.515	1.519	1.522	1.523	1.522
SiS	1.929	1.951	1.937	1.937	1.941	1.941	1.941
P_2	1.893	1.905	1.891	1.892	1.897	1.897	1.896
P_4	2.210	2.208	2.190	2.193	2.197	2.195	2.194
PH	1.421	1.440	1.427	1.424	1.43	1.434	1.435
PF	1.589	1.617	1.599	1.607	1.606	1.605	1.604
PCl	2.015	2.031	2.019	2.021	2.022	2.019	2.018
PN	1.491	1.500	1.487	1.492	1.497	1.496	1.496
PO	1.476	1.497	1.482	1.488	1.49	1.491	1.491
S_2	1.889	1.912	1.896	1.900	1.903	1.902	1.901
SH	1.341	1.356	1.345	1.342	1.351	1.353	1.353
SF	1.601	1.622	1.605	1.617	1.614	1.611	1.611
SF_6	1.561	1.596	1.576	1.589	1.588	1.586	1.585
SO	1.481	1.505	1.490	1.499	1.502	1.502	1.501
SO_3	1.420	1.444	1.429	1.438	1.443	1.441	1.441
Cl_2	1.988	2.008	1.996	2.005	1.999	1.998	1.997
Cl_2^+	1.891	1.914	1.898	1.908	1.907	1.904	1.904
HCl	1.275	1.288	1.279	1.277	1.285	1.287	1.287
HCl^+	1.315	1.333	1.321	1.319	1.326	1.329	1.329
ClF	1.628	1.652	1.636	1.651	1.644	1.642	1.641
ClO	1.570	1.583	1.575	1.587	1.587	1.582	1.581
ME		0.018	0.005	0.008	0.014	0.011	0.013
MAD		0.018	0.010	0.011	0.014	0.012	0.014
Spread		0.168	0.183	0.197	0.182	0.069	0.180

(continued)

TABLE III: Harmonic vibrational frequencies in cm^{-1} for the T82-F molecular test set [3, 4] obtained with different approximate exchange-correlation functionals.

Molecule	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC_{opt}	RPP	SRPP	SRPP2
H_2	4401.20	4316.60	4429.67	4433.00	4371.53	4327.35	4324.43
Li_2	351.40	329.83	332.37	338.50	338.47	333.75	332.84
LiH	1405.70	1377.44	1394.28	1398.39	1396.20	1371.50	1370.36
LiF	910.60	894.04	904.77	900.09	885.08	897.14	897.40
LiCl	643.00	644.19	642.66	647.69	634.26	645.30	645.29
LiO	814.60	797.92	810.73	805.43	787.24	799.84	800.45
LiNa	256.80	245.92	246.33	249.04	252.01	247.52	247.07
Be_2	267.90	347.20	327.20	378.91	346.68	343.15	349.11
BeH	2060.80	1974.63	2009.73	2032.61	2009.19	1984.28	1982.27
BeH^+	2221.70	2109.72	2203.03	2204.43	2198.05	2154.33	2149.43
BeF	1247.40	1196.15	1222.55	1216.82	1218.48	1228.28	1202.22
BeCl	846.70	809.36	816.44	828.52	810.65	820.71	815.07
BeO	1487.30	1455.69	1508.31	1485.15	1456.67	1487.07	1461.34
BeS	997.90	975.83	1008.22	1002.21	979.79	987.75	982.77
B_2	1051.30	1011.60	1012.77	1026.00	983.66	992.61	998.80
BH	2366.90	2245.71	2301.01	2311.73	2256.06	2227.03	2229.62
BF	1402.10	1354.73	1398.46	1374.72	1342.91	1385.58	1359.25
BCl	840.30	810.20	826.55	822.02	794.66	807.44	809.30
BN	1514.60	1513.24	1570.16	1547.01	1490.76	1499.27	1506.61
BO	1885.70	1844.00	1896.33	1866.83	1827.00	1836.68	1839.49
BS	1180.20	1161.49	1195.46	1185.04	1154.00	1164.01	1166.19
C_2	1854.70	1857.11	1891.01	1873.68	1814.53	1845.67	1851.12
CH	2858.50	2730.18	2803.97	2802.58	2717.51	2703.82	2711.20
CF	1308.10	1257.32	1297.42	1257.20	1267.71	1258.92	1262.54
CN	2068.60	2093.57	2149.60	2113.03	2052.96	2078.42	2082.69
CO	2169.80	2129.62	2195.55	2145.55	2102.96	2120.42	2123.10
CO^+	2214.20	2202.58	2277.95	2226.89	2167.03	2189.17	2193.61
CP	1239.70	1250.18	1286.41	1269.35	1243.47	1252.93	1256.44
CS	1285.20	1263.69	1304.75	1279.88	1250.36	1265.86	1267.51
N_2	2358.60	2353.66	2432.68	2371.77	2322.33	2347.03	2349.06
N_2^+	2207.00	2264.91	2326.82	2282.72	2221.04	2251.81	2255.96
NH	3282.30	3171.82	3246.50	3217.63	3169.81	3147.40	3152.57
NF	1141.40	1128.53	1171.33	1122.99	1147.68	1158.61	1151.40
NCl	828.00	835.85	836.47	823.16	819.27	829.28	832.01
NO	1904.20	1892.16	1959.47	1893.38	1860.06	1885.39	1888.07
NO^+	2376.40	2363.83	2456.14	2379.66	2332.54	2357.53	2359.95
NS	1218.70	1213.17	1254.42	1220.84	1202.44	1214.74	1216.54
O_2	1580.20	1555.90	1624.96	1552.32	1543.40	1564.41	1566.14
O_2^+	1904.80	1931.33	2026.58	1932.96	1910.89	1934.72	1937.02
OH	3737.80	3602.70	3718.29	3689.78	3586.13	3603.59	3610.53
OH^+	3113.40	2953.36	3060.89	3023.95	3013.58	2983.14	2981.67
F_2	916.60	997.29	1048.14	1006.03	1031.52	1038.01	1038.14
F_2^+	1073.30	1151.83	1219.83	1154.32	1184.86	1191.36	1191.37
HF	4138.30	3977.20	4093.34	4047.58	3992.40	3994.60	3997.35
HF^+	3090.50	2910.03	3024.75	3000.15	2969.50	2984.50	2982.06

(continued)

Na_2	159.10	158.96	155.29	156.89	159.67	156.37	156.40
NaH	1172.20	1143.28	1167.88	1170.47	1165.63	1156.85	1155.25
NaF	535.70	519.85	539.36	533.81	526.42	535.24	535.30
NaO	492.30	466.16	488.05	483.38	476.89	492.98	480.81
MgH	1495.20	1409.21	1461.59	1480.39	1446.46	1442.57	1440.94
MgH^+	1699.10	1642.69	1720.88	1721.29	1710.40	1686.19	1684.64
MgO	784.80	803.21	837.42	823.41	817.03	821.12	821.86
MgS	528.70	526.22	550.24	543.50	536.33	539.89	540.49
Al_2	350.00	341.93	355.77	354.35	346.17	351.23	351.82
AlH	1682.60	1585.99	1646.51	1651.24	1640.49	1619.27	1617.47
AlF	802.30	747.66	788.75	776.71	778.51	775.25	775.60
AlCl	481.30	458.80	475.87	473.41	473.17	473.04	473.35
AlO	979.20	956.88	992.26	985.14	968.91	977.86	979.49
AlS	617.10	600.43	630.55	625.83	614.65	618.91	619.80
Si_2	511.00	483.24	564.20	499.32	494.77	496.11	496.47
SiH	2041.80	1951.71	2020.24	2030.81	2000.44	1988.65	1991.73
SiH^+	2157.20	2047.83	2119.64	2110.97	2097.12	2075.18	2074.57
SiF	857.20	807.65	847.30	831.01	829.59	833.84	834.51
SiCl	535.60	515.10	529.27	524.43	519.68	525.31	526.11
SiN	1151.40	1150.13	1179.68	1166.46	1153.27	1159.34	1161.35
SiO	1241.50	1196.56	1247.89	1219.92	1211.37	1214.75	1215.29
SiS	749.60	726.42	753.33	741.63	732.90	737.80	738.11
P_2	780.80	782.42	813.84	798.52	788.15	793.89	794.29
P_2^+	672.20	674.31	707.78	693.66	682.77	687.62	688.41
PH	2365.20	2288.59	2367.90	2363.18	2334.76	2325.82	2328.34
PF	846.80	811.02	846.90	821.17	830.54	833.92	834.37
PCl	551.40	538.06	550.12	539.08	536.18	545.71	546.02
PN	1337.20	1339.51	1390.71	1357.51	1338.92	1347.00	1347.93
PO	1233.30	1200.39	1250.59	1214.09	1206.29	1213.16	1213.74
S_2	725.60	701.88	732.65	713.94	712.11	716.22	716.63
SO	1149.20	1110.40	1159.28	1115.80	1107.97	1120.40	1121.32
Cl_2	559.70	540.40	555.49	535.88	547.72	549.42	549.81
Cl_2^+	645.60	624.21	649.26	629.91	639.71	643.79	644.28
HCl	2990.90	2901.24	2981.86	2965.12	2914.08	2912.64	2916.91
HCl^+	2673.70	2571.65	2643.90	2630.45	2600.05	2587.48	2587.86
ClF	786.10	760.84	791.24	758.60	779.22	781.65	782.01
ClO	853.80	862.59	872.53	843.62	852.22	866.65	868.68
ME		-33.781	11.336	-7.248	-26.743	-22.875	-22.945
MAD		43.613	30.899	25.709	36.711	36.134	36.800
Spread		261.16	212.42	201.73	266.59	276.09	268.84

II. SOLID TEST SET RESULTS

Here we provide the solid-by-solid tabulation for the KS (or gKS) band gaps (21 systems), equilibrium lattice constants and cohesive energies (55 solids), and bulk moduli (44 cubic solids) for r^{2}SCAN-L(SRPP) and r^{2}SCAN-L(SRPP2) compared r^{2}SCAN-L(RPP), r^{2}SCAN-L(PC$_{opt}$), r^{2}SCAN, and PBE. These calculations were done with VASP 5.4.4.

TABLE IV. Equilibrium lattice constants, $a_0(\AA)$ compared for 55 solids. Experimental values Exptl. are from Ref. [5], include zero-point effects.

Solid	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC$_{opt}$	RPP	SRPP	SRPP2
C	3.553	3.572	3.562	3.569	3.578	3.573	3.572
Si	5.421	5.469	5.440	5.429	5.431	5.428	5.427
Ge	5.644	5.782	5.681	5.709	5.689	5.673	5.676
Sn	6.477	6.653	6.565	6.593	6.533	6.532	6.531
SiC	4.346	4.379	4.355	4.356	4.370	4.365	4.364
BN	3.592	3.626	3.614	3.619	3.629	3.625	3.625
BP	4.525	4.547	4.533	4.538	4.542	4.539	4.538
AlN	4.368	4.402	4.368	4.366	4.380	4.374	4.373
AlP	5.451	5.506	5.472	5.463	5.470	5.465	5.464
AlAs	5.649	5.733	5.677	5.678	5.671	5.668	5.663
GaN	4.520	4.589	4.527	4.548	4.546	4.541	4.540
GaP	5.439	5.534	5.467	5.485	5.470	5.464	5.464
GaAs	5.640	5.762	5.672	5.701	5.668	5.666	5.665
InP	5.858	6.001	5.947	5.948	5.935	5.928	5.927
InAs	6.047	6.211	6.131	6.151	6.112	6.109	6.108
InSb	6.468	6.647	6.569	6.581	6.535	6.530	6.527
LiH	3.979	4.016	4.012	3.988	4.020	4.010	4.010
LiF	3.972	4.071	3.994	4.003	4.009	4.004	4.004
LiCl	5.070	5.153	5.111	5.079	5.069	5.063	5.063
NaF	4.582	4.632	4.503	4.508	4.524	4.518	4.513
NaCl	5.569	5.655	5.545	5.519	5.519	5.517	5.512
MgO	4.189	4.248	4.196	4.192	4.191	4.187	4.187
Li	3.443	3.439	3.479	3.432	3.458	3.461	3.462
Na	4.214	4.193	4.200	4.140	4.151	4.151	4.151
K	5.212	5.286	5.350	5.264	5.228	5.231	5.229
Rb	5.577	5.669	5.751	5.667	5.631	5.605	5.594
Cs	6.039	6.161	6.271	6.177	6.121	6.061	6.103
Ca	5.556	5.525	5.574	5.503	5.512	5.502	5.499
Ba	5.002	5.030	5.077	5.054	5.001	4.968	4.975
Sr	6.040	6.027	6.101	6.048	6.021	6.007	6.007
Al	4.018	4.040	3.988	3.977	3.993	3.991	3.990
Fe	2.853	2.829	2.865	2.854	2.797	2.794	2.794
Co	3.524	3.517	3.514	3.516	3.469	3.467	3.467
Ni	3.508	3.518	3.479	3.507	3.469	3.467	3.467
Sc	3.270	3.249	3.260	3.226	3.225	3.222	3.222
Y	3.594	3.592	3.623	3.601	3.579	3.574	3.574
Ti	2.915	2.893	2.887	2.877	2.868	2.866	2.866
Zr	3.198	3.210	3.215	3.216	3.189	3.188	3.188
Hf	3.151	3.158	3.141	3.150	3.126	3.126	3.126
V	3.021	2.978	2.965	2.965	2.949	2.948	2.948
Nb	3.294	3.322	3.320	3.322	3.297	3.295	3.295
Ta	3.299	3.309	3.290	3.301	3.277	3.276	3.276
Mo	3.141	3.151	3.144	3.149	3.128	3.127	3.127
W	3.160	3.172	3.156	3.167	3.147	3.146	3.146
Tc	2.716	2.725	2.716	2.723	2.703	2.702	2.702
Re	2.744	2.764	2.750	2.760	2.742	2.742	2.742
Ru	2.669	2.683	2.672	2.683	2.659	2.659	2.659
Os	2.699	2.723	2.708	2.723	2.703	2.703	2.703
Rh	3.794	3.824	3.804	3.824	3.783	3.782	3.782
Ir	3.831	3.872	3.852	3.877	3.839	3.839	3.839
Pd	3.876	3.939	3.912	3.938	3.881	3.881	3.881
Pt	3.913	3.968	3.943	3.974	3.925	3.924	3.924
Cu	3.595	3.634	3.582	3.611	3.566	3.567	3.567
Ag	4.062	4.147	4.108	4.141	4.067	4.066	4.067
Au	4.062	4.156	4.128	4.167	4.097	4.095	4.095
ME		0.046	0.026	0.022	0.003	-0.003	-0.002
MAD		0.053	0.037	0.038	0.029	0.028	0.028
Spread		0.222	0.311	0.212	0.154	0.143	0.142

TABLE V. Cohesive energies, $E_{coh}(eV/atom)$ of 55 solids. Experimental values Exptl. are from Ref. [5]. They include zero-point effects.

Solid	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC_{opt}	RPP	SRPP	SRPP2
C	7.550	7.714	7.467	7.354	7.376	7.563	7.611
Si	4.680	4.561	4.675	4.498	4.584	4.712	4.733
Ge	3.890	3.725	3.891	3.534	3.884	3.943	3.957
Sn	3.160	3.200	3.295	3.076	3.323	3.364	3.370
SiC	6.480	6.408	6.432	6.231	6.266	6.418	6.455
BN	6.760	6.936	6.788	6.704	6.636	6.803	6.857
BP	5.140	5.293	5.281	5.141	5.161	5.319	5.357
AlN	5.850	5.711	5.809	5.717	5.631	5.739	5.779
AlP	4.320	4.093	4.249	4.137	4.169	4.266	4.288
AlAs	3.820	3.693	3.867	3.683	3.812	3.889	3.907
GaN	4.550	4.385	4.465	4.308	4.429	4.493	4.519
GaP	3.610	3.478	3.642	3.444	3.637	3.706	3.718
GaAs	3.340	3.161	3.328	3.066	3.344	3.390	3.398
InP	3.470	3.123	3.245	3.103	3.285	3.346	3.357
InAs	3.080	2.893	3.026	2.812	3.071	3.113	3.120
InSb	2.810	2.650	2.729	2.580	2.773	2.814	2.821
LiH	2.490	2.348	2.420	2.420	2.359	2.372	2.378
LiF	4.460	4.321	4.395	4.293	4.189	4.275	4.288
LiCl	3.590	3.352	3.467	3.403	3.325	3.393	3.404
NaF	3.970	3.860	3.992	3.875	3.779	3.859	3.875
NaCl	3.340	3.088	3.260	3.177	3.098	3.161	3.172
MgO	5.200	4.998	5.249	5.141	5.005	5.126	5.159
Li	1.670	1.600	1.569	1.606	1.563	1.584	1.592
Na	1.120	1.038	1.041	1.017	1.025	1.044	1.049
K	0.940	0.857	0.841	0.826	0.823	0.838	0.848
Rb	0.860	0.760	0.734	0.734	0.739	0.750	0.759
Cs	0.810	0.693	0.661	0.626	0.650	0.662	0.669
Ca	1.870	1.846	1.917	1.986	1.981	2.039	2.034
Ba	1.910	1.703	1.817	1.858	1.894	1.927	1.930
Sr	1.730	1.604	1.786	1.729	1.802	1.805	1.817
Al	3.430	3.442	3.609	3.437	3.456	3.562	3.589
Fe	4.300	4.871	4.635	4.529	4.819	4.994	5.020
Co	4.420	5.165	4.871	4.450	5.052	5.152	5.163
Ni	4.480	4.732	4.645	4.320	4.910	4.981	4.988
Sc	3.930	4.142	4.017	3.874	4.060	4.148	4.166
Y	4.390	4.100	4.014	3.771	4.019	4.095	4.108
Ti	4.880	5.442	5.060	5.104	5.213	5.412	5.420
Zr	6.270	5.344	4.378	4.658	5.271	5.294	5.277
Hf	6.460	6.455	6.434	6.058	6.438	6.525	6.535
V	5.350	6.520	4.660	4.818	5.340	5.419	5.426
Nb	7.600	6.919	6.361	6.189	6.968	6.992	6.975
Ta	8.130	8.314	8.251	7.732	8.422	8.470	8.478
Mo	6.860	6.351	5.690	5.635	6.551	6.563	6.563
W	8.940	8.485	8.067	7.631	8.554	8.557	8.558
Tc	6.880	6.971	6.337	6.175	7.068	7.147	7.155
Re	8.050	7.815	7.514	7.166	8.147	8.192	8.202
Ru	6.770	6.773	6.338	6.040	6.834	6.974	6.993
Os	8.200	8.356	8.072	7.530	8.651	8.717	8.725
Rh	5.780	5.748	5.826	5.287	6.184	6.232	6.240
Ir	6.990	7.494	7.142	6.557	7.717	7.787	7.798
Pd	3.930	3.738	4.163	3.696	4.290	4.275	4.279
Pt	5.870	5.531	5.716	5.067	5.972	6.008	6.014
Cu	3.510	3.479	3.855	3.487	3.865	3.884	3.891
Ag	2.960	2.511	2.873	2.484	2.895	2.912	2.918
Au	3.830	3.033	3.417	2.918	3.465	3.495	3.502
ME		-0.070	-0.134	-0.327	-0.017	0.051	0.064
MAD		0.252	0.238	0.349	0.217	0.224	0.227
Spread		2.096	2.343	1.841	1.726	1.773	1.801

TABLE VI. Bulk modulus, $B_0(GPa)$ of 44 cubic solids. Experimental values Exptl. are from Ref. [6]. Theoe values were obtained by subtracting the zero-point phonon effect from the experimental zero-temperature values.

Solid	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC$_{opt}$	RPP	SRPP	SRPP2
C	454.700	433.061	449.244	433.521	426.102	434.550	434.752
Si	101.300	88.798	97.272	93.345	93.027	94.828	94.926
Ge	79.400	59.083	73.095	68.252	69.444	72.097	71.137
Sn	42.800	36.172	43.526	39.541	43.056	43.295	43.404
SiC	229.100	212.361	226.927	219.406	217.076	218.734	219.177
BN	410.200	372.412	389.901	377.584	371.004	375.865	375.887
BP	168.000	161.851	170.052	165.254	163.423	165.806	165.776
AlN	206.000	193.670	212.380	207.043	203.591	205.484	205.858
AlP	87.400	82.678	91.095	88.727	86.863	88.013	88.187
AlAs	75.000	67.252	76.387	73.888	74.033	74.514	77.984
GaN	213.000	182.466	211.373	197.740	199.732	201.902	202.134
GaP	89.600	78.712	90.466	87.722	85.754	87.561	90.244
GaAs	76.700	62.019	73.804	69.055	72.266	72.274	72.460
InP	72.000	60.930	70.286	66.749	68.827	69.057	69.137
InAs	58.600	49.497	58.929	56.038	58.385	58.702	58.715
InSb	46.100	37.074	44.017	40.168	43.914	43.993	45.254
LiH	40.100	36.343	36.485	38.008	38.688	37.347	37.878
LiF	76.300	67.393	78.714	78.913	71.336	75.796	76.121
LiCl	38.700	31.863	35.064	37.084	37.279	37.152	37.230
NaF	53.100	47.016	59.895	59.433	59.036	58.120	58.677
NaCl	27.600	24.264	29.140	31.114	28.192	29.053	29.183
MgO	169.800	151.596	170.619	170.667	168.916	170.047	170.184
Li	13.100	13.957	13.116	14.902	13.929	14.043	13.922
Na	7.900	7.877	7.930	8.527	8.453	8.493	8.507
K	3.800	3.593	3.422	3.981	3.901	3.886	3.913
Rb	3.600	2.798	2.631	2.688	3.201	2.976	2.914
Cs	2.300	1.960	1.867	2.486	2.269	2.850	3.528
Ca	15.900	17.458	17.595	19.379	19.370	19.248	19.285
Ba	10.600	8.844	8.569	10.071	10.076	8.990	11.024
Sr	12.000	11.598	11.832	11.853	13.017	12.609	12.650
Al	77.100	77.996	92.466	90.178	89.622	89.701	89.910
Ni	192.500	196.258	216.804	240.644	221.814	221.519	221.721
V	165.800	187.488	201.269	200.164	208.244	207.710	207.734
Nb	173.200	173.453	178.078	176.731	182.676	183.427	183.441
Ta	202.700	201.055	210.119	208.545	213.389	213.655	213.661
Mo	276.200	268.535	281.995	269.301	287.044	287.799	287.823
W	327.500	312.477	329.918	316.703	331.947	332.637	332.679
Rh	277.100	258.115	281.584	257.708	290.794	291.526	291.553
Ir	362.200	349.818	378.905	343.185	385.920	386.156	386.134
Pd	187.200	169.148	186.087	165.311	199.522	199.564	199.567
Pt	285.500	249.877	273.641	243.359	282.471	283.503	283.516
Cu	144.300	138.007	159.969	146.405	168.178	167.601	167.609
Ag	105.700	90.318	103.562	92.107	111.352	111.615	111.495
Au	182.000	139.596	153.795	133.245	164.250	164.826	164.835
ME		-9.704	1.367	-4.249	1.084	1.928	2.228
MAD		11.022	5.963	10.115	8.542	7.866	7.851
Spread		64.092	63.674	96.899	81.64	76.245	76.247

TABLE VII. 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. [7].

Solid	Exptl	PBE	r^{2}SCAN	r^{2}SCAN-L			
				PC$_{opt}$	RPP	SRPP	SRPP2
C	5.50	4.13	4.32	4.23	4.07	4.06	4.06
Si	1.17	0.58	0.78	0.83	0.70	0.67	0.67
Ge	0.74	0.09	0.50	0.35	0.21	0.27	0.27
SiC	2.42	1.38	1.75	1.69	1.42	1.46	1.46
BN	6.36	4.48	5.00	4.81	4.50	4.51	4.51
BP	2.10	1.24	1.45	1.42	1.30	1.26	1.26
AlN	4.90	3.35	3.97	3.73	3.47	3.50	3.50
AlP	2.50	1.59	1.92	1.88	1.68	1.68	1.68
AlAs	2.23	1.44	1.80	1.73	1.59	1.58	1.58
GaN	3.28	1.74	2.19	1.90	1.71	1.80	1.81
GaP	2.35	1.62	1.89	1.86	1.70	1.70	1.70
GaAs	1.52	0.61	1.09	0.90	0.78	0.81	0.81
InP	1.42	0.75	1.18	1.01	0.85	0.89	0.89
InAs	0.42	0.00	0.25	0.12	0.02	0.04	0.04
InSb	0.24	0.00	0.27	0.16	0.07	0.07	0.07
LiH	4.94	3.07	3.72	3.60	3.46	3.36	3.34
LiF	14.20	9.20	10.19	9.66	9.22	9.32	9.34
LiCl	9.40	6.41	7.31	6.97	6.62	6.67	6.67
NaF	11.50	6.37	7.21	6.70	6.34	6.40	6.42
NaCl	8.50	5.19	5.98	5.67	5.34	5.39	5.39
MgO	7.83	4.77	5.65	5.28	4.91	5.02	5.03
ME		-1.69	-1.20	-1.38	-1.60	-1.58	-1.57
MAD		1.69	1.20	1.38	1.60	1.58	1.57
Spread		4.888	4.317	4.717	4.988	4.93	4.918

III. TIMES IN MOLECULES CALCULATED IN NWCHEM-7.0.2

Here we provide the total time and the number of SCF cycles for each molecule from the G3X/99 test set calculated with r^{2}SCAN-L(SRPP) and r^{2}SCAN-L(SRPP2) compared r^{2}SCAN-L(RPP), r^{2}SCAN-L(PC$_{opt}$), r^{2}SCAN, and PBE. Calculations from this section were performed with NWChem-7.0.2.

TABLE VIII: Timing in seconds required for computing each of the molecules in the G3X/99 test set.

Molecule	r^{2}SCAN	r^{2}SCAN-L				PBE
		PC$_{opt}$	RPP	SRPP	SRPP2	
LiH	2.8	0.6	1.6	0.9	0.5	0.9
^{2}BeH	1.4	0.8	1.7	1.1	0.7	0.8
^{2}CH	1.3	1.1	1.7	2.3	1.0	0.7
CH_2 ($^3B_1$)	2.3	1.5	2.0	1.6	1.1	0.8
CH_2 ($^1A_1$)	1.1	1.1	1.6	1.1	0.9	0.6
$^3CH_3$	1.9	2.3	3.0	2.1	1.5	1.0
CH_4	1.9	1.9	3.4	2.4	1.5	1.3
^{3}NH	0.9	1.3	2.1	1.7	0.9	0.6
NH_2 ($^2B_1$)	1.3	2.6	3.2	1.6	1.2	0.9
NH_3	1.6	1.1	1.2	1.2	1.1	0.8
^{2}OH	2.2	0.9	1.2	1.0	1.0	0.8
H_2O	1.8	0.8	1.0	0.8	0.8	0.7
HF	1.4	0.6	1.6	1.0	0.9	0.7
SiH_2 ($^1A_1$)	2.2	1.0	1.5	1.1	1.1	1.1
SiH_2 ($^3B_1$)	2.1	1.9	2.6	1.6	1.7	1.1
$^2SiH_3$	2.4	2.1	3.8	2.0	1.8	1.5
SiH_4	2.3	1.5	2.6	2.3	1.8	1.3
$^2PH_2$	2.2	1.7	3.7	2.7	1.6	1.0
PH_3	2.6	1.2	6.5	1.6	1.4	0.9
H_2S	2.5	1.2	2.3	1.4	1.1	0.8
HCl	1.7	0.8	2.4	1.2	0.8	0.6
Li_2	1.0	0.5	1.2	1.2	0.5	0.5
LiF	1.3	0.8	1.7	1.5	0.7	0.8
HC≡CH	1.5	1.3	1.9	2.6	1.2	0.9
$H_2C{=}CH_2$	3.4	2.5	3.7	3.0	2.4	2.0
$H_3C{-}CH_3$	4.4	3.7	5.8	4.4	3.5	2.0
CN	4.2	1.9	2.8	2.0	2.0	1.0
HCN	2.6	1.4	3.3	1.9	1.1	1.0
CO	2.1	1.1	2.2	1.0	0.8	0.8
^{2}HCO	3.4	1.9	3.5	2.4	1.8	1.0
H_2CO	1.7	1.8	2.5	2.1	1.3	1.0
CH_3OH	3.3	3.1	5.2	3.1	3.0	1.6
N_2	0.9	0.7	1.4	1.9	1.7	0.8
H_2NNH_2	2.9	2.8	4.6	3.3	2.8	2.0
NO	1.9	1.3	2.1	1.6	1.2	1.2
$^3O_2$	1.6	1.6	2.5	1.6	1.3	0.7
H_2O_2	1.8	1.4	2.4	2.7	1.5	1.2
F_2	1.4	0.8	1.7	1.5	0.8	0.7
CO_2	1.6	1.7	3.2	1.9	1.2	0.9
Na_2	1.3	0.9	2.5	1.5	1.1	0.7
Si_2	3.5	4.1	5.3	3.8	3.6	1.8
P_2	1.7	1.2	2.6	2.0	1.7	1.1
$^3S_2$	2.4	2.3	3.6	2.6	2.1	1.3

(continued)

Cl_2	1.7	1.2	2.0	2.0	1.3	0.8
NaCl	2.0	1.4	3.2	1.9	1.3	1.2
SiO	2.2	1.2	2.2	1.6	1.4	1.0
CS	1.7	1.6	2.4	1.7	1.3	1.0
SO	2.6	3.2	3.3	2.9	2.4	1.3
ClO	2.3	2.9	3.3	2.8	3.5	2.3
ClF	1.6	1.7	2.4	1.9	1.9	1.2
Si_2H_6	4.4	4.9	6.5	5.5	5.0	2.4
CH_3Cl	2.9	3.1	4.2	2.9	2.7	1.5
H_3C-SH	3.9	3.4	5.2	3.5	4.0	1.9
HOCl	1.8	1.8	2.1	2.5	1.4	1.1
SO_2	2.1	2.0	2.9	2.0	1.8	1.1
BF_3	3.1	2.2	3.8	2.1	1.8	1.4
BCl_3	3.5	3.7	4.7	3.0	2.7	2.1
AlF_3	3.1	2.4	3.9	2.1	1.8	1.5
$AlCl_3$	3.3	3.1	5.7	3.7	3.2	2.2
CF_4	3.6	3.5	3.9	3.8	3.0	2.0
CCl_4	5.7	5.0	6.6	7.3	5.4	3.2
OCS	2.8	2.5	3.1	2.4	2.5	1.5
CS_2	2.1	2.2	3.5	3.6	1.9	1.3
F_2CO	2.6	2.9	3.1	2.5	2.3	1.6
SiF_4	3.6	3.6	4.1	3.3	3.0	2.0
$SiCl_4$	6.2	6.9	6.7	6.0	4.9	3.3
NNO	2.8	1.8	2.6	3.1	2.2	1.4
ClNO	7.8	6.8	9.1	6.1	5.7	3.2
NF_3	2.8	2.5	3.7	2.4	2.2	1.9
PF_3	2.7	2.3	4.1	3.2	2.5	1.4
O_3	2.1	2.2	2.5	2.2	2.3	1.0
F_2O	2.6	1.7	2.5	2.2	1.4	1.5
ClF_3	3.6	3.5	4.1	3.0	5.3	3.2
$F_2C=CF_2$	10.0	5.7	6.4	5.3	5.0	2.7
$Cl_2C=CCl_2$	8.0	9.1	9.6	7.5	7.3	4.3
F_3C-CN	7.4	9.2	9.9	8.7	7.5	4.2
$HC\equiv C-CH_3$	4.5	5.4	8.1	5.0	4.4	2.3
$H_2C=C=CH_2$	4.7	4.7	5.8	4.5	3.8	2.1
C_3H_4 (cyclopropene)	4.5	5.1	7.4	4.5	4.3	2.1
$H_2C=CH-CH_3$	6.7	7.2	9.7	6.8	5.8	3.1
C_3H_6 (cyclopropane)	5.6	6.7	9.2	6.2	6.1	3.0
$CH_3-CH_2-CH_3$	8.3	9.4	10.5	9.1	8.3	4.6
C_4H_6 (Z-1,3-butadiene)	7.4	9.2	11.4	8.8	8.5	3.9
C_4H_6 (2-butyne)	7.2	10.6	14.2	7.2	7.2	3.9
C_4H_6 (methylenecyclopropane)	8.3	11.6	12.8	9.7	9.7	4.6
C_4H_6 (bicyclo[1.1.0]butane)	9.0	11.5	12.6	9.8	9.1	4.8
C_4H_6 (cyclobutene)	7.5	9.9	12.8	9.6	8.6	4.7
C_4H_8 (cyclobutane)	10.2	12.7	15.1	12.5	12.3	6.6
C_4H_8 (isobutene)	10.7	15.0	16.3	12.2	11.0	7.0
C_4H_{10} (trans butane)	14.5	18.8	21.3	14.9	14.5	8.1
C_4H_{10} (isobutane)	15.0	19.7	24.3	17.4	15.2	8.5
C_5H_8 (spiropentane)	15.2	19.2	19.0	15.4	15.1	8.9
C_6H_6 (benzene)	15.5	24.3	20.1	16.2	18.0	8.7
CH_2F_2	2.3	3.0	5.0	3.3	2.5	1.8
CHF_3	3.0	3.8	5.0	3.4	2.9	1.7

(continued)

CH_2Cl_2	3.9	4.3	4.2	3.7	3.1	3.8
$CHCl_3$	4.5	5.6	6.2	5.0	4.6	2.6
CH_3NH_2	3.4	4.8	5.8	4.0	3.5	2.1
CH_3CN	3.3	5.1	5.4	4.8	3.7	2.3
CH_3NO_2 (nitromethane)	8.1	7.3	8.8	7.0	7.2	4.2
CH_3ONO (methyl nitrite)	6.6	6.8	7.5	6.5	6.4	4.0
CH_3SiH_3	6.0	3.9	5.3	4.4	4.6	4.1
HCO_2H	4.8	3.2	3.9	3.1	3.2	2.0
HCO_2CH_3	7.4	6.2	8.5	7.4	6.3	3.6
CH_3CONH_2	11.2	10.1	10.8	9.2	9.4	5.3
C_2H_5N (aziridine)	7.0	5.8	6.8	6.6	5.6	4.6
NCCN (cyanogen)	2.8	2.0	2.2	2.1	2.2	1.8
$NH(CH_3)_2$	8.8	8.7	9.7	9.3	8.5	5.2
$CH_3CH_2NH_2$	11.3	7.8	10.4	7.7	8.0	5.0
$H_2C{=}C{=}O$ (ketene)	5.7	3.4	4.0	3.7	3.5	2.6
C_2H_4O (oxirane)	5.3	4.7	5.8	3.9	4.0	6.6
CH_3CHO	6.9	5.1	5.9	5.3	5.2	3.2
$O{=}CH{-}CH{=}O$	4.5	3.7	5.1	3.7	4.1	2.3
CH_3CH_2OH	6.6	6.1	9.2	5.8	5.9	4.4
$(CH_3)_2O$	8.5	6.2	9.3	6.4	6.1	3.4
C_2H_4S (thiooxirane)	6.0	5.1	6.2	5.2	5.2	3.0
$(CH_3)_2S{=}O$	13.4	12.3	14.0	12.1	11.7	6.6
CH_3CH_2SH	8.7	7.2	8.9	7.5	7.5	4.2
$(CH_3)_2S$	7.8	6.5	7.7	6.2	6.5	3.6
$H_2C{=}CHF$	4.4	3.5	4.4	4.5	4.0	2.4
CH_3CH_2Cl	6.3	5.5	8.7	6.1	6.1	3.5
$H_2C{=}CHCl$	5.6	4.5	5.4	4.2	4.0	2.8
$H_2C{=}CHCN$	7.7	5.7	8.6	6.8	6.5	3.9
$(CH_3)_2C{=}O$	11.1	8.7	12.9	9.5	9.6	5.1
CH_3CO_2H	9.4	7.6	10.3	7.6	7.5	4.5
CH_3CFO	5.8	6.6	8.2	6.9	6.7	3.9
CH_3COCl	8.0	7.5	9.0	7.3	7.6	4.9
$CH_3CH_2CH_2Cl$	10.8	10.4	14.2	11.6	11.8	6.4
$(CH_3)_2CHOH$	12.3	13.2	15.9	13.0	12.7	7.3
$CH_3{-}O{-}CH_2CH_3$	11.5	10.4	17.5	11.9	11.8	6.7
$(CH_3)_3N$	14.5	15.4	18.8	15.7	15.4	8.8
C_4H_4O (furan)	10.3	9.7	11.7	9.9	9.5	6.6
C_4H_4S (thiophene)	11.8	12.9	13.1	10.9	10.3	7.3
C_4H_5N (pyrrole)	11.9	14.7	16.7	14.0	13.7	7.6
C_5H_5N (pyridine)	18.8	17.9	20.4	17.5	17.9	10.6
H_2	1.8	0.5	1.2	0.6	0.4	0.6
^2SH	1.9	2.3	1.5	1.2	1.3	1.3
$^2C{\equiv}CH$	4.0	3.6	6.1	3.2	3.3	1.7
$HC{=}CH_2$ ($^2A''$)'	6.7	5.7	6.4	5.3	5.1	2.6
$CH_3C{=}O$ ($^2A''$)'	8.5	8.0	8.5	7.7	7.7	3.8
$CH_2{-}OH$ (^2A)	4.6	4.0	4.3	4.0	4.4	2.5
CH_3O ($^2A''$)'	4.7	4.2	4.7	4.2	4.1	3.7
CH_3CH_2O ($^2A''''$)'	9.5	9.3	11.3	20.2	19.5	9.9
CH_3S ($^2A''$)'	5.4	5.2	4.6	5.8	5.7	2.9
CH_2CH_3 ($^2A''$)'	6.2	5.6	6.1	5.3	5.6	2.7
$(CH_3)_2CH$ ($^2A''$)'	14.7	14.2	14.9	13.9	14.2	6.3
$^2C(CH_3)_3$	26.1	25.7	29.9	26.2	26.0	12.3

(continued)

NO_2 ($^2A_1$)	2.7	2.3	2.5	2.4	2.1	1.5
$CH_3CH{=}C{=}CH_2$	11.2	10.6	12.7	11.8	11.1	5.5
C_5H_8 (isoprene)	21.0	19.8	23.2	20.5	21.4	10.8
C_5H_{10} (cyclopentane twist)	18.8	17.9	24.7	20.8	20.3	11.5
C_5H_{12} (n-pentane)	21.5	17.9	28.7	20.9	20.6	13.7
$C(CH_3)_4$ (neopentane)	26.0	28.7	35.0	24.8	25.8	14.1
C_6H_8 (1,3-cyclohexadiene)	19.0	22.3	26.0	21.6	21.8	12.3
C_6H_8 (1,4-cyclohexadiene)	19.6	21.6	25.1	21.5	21.8	12.2
C_6H_{12} (cyclohexane chair)	30.6	30.8	36.3	30.3	30.1	17.6
C_6H_{14} (n-hexane)	28.5	24.3	40.0	32.2	31.6	18.6
C_6H_{14} (3-methylpentane)	33.6	37.9	46.1	37.7	38.2	21.3
$C_6H_5{-}CH_3$ (toluene)	29.6	35.9	43.2	35.3	35.3	22.0
C_7H_{16} (n-heptane)	42.6	40.7	49.2	41.1	40.6	24.4
C_8H_8 (cyclooctatetraene)	59.4	65.7	38.3	31.8	31.6	18.8
C_8H_{18} (n-octane)	51.2	50.8	60.2	50.0	49.7	30.6
$C_{10}H_8$ (naphtalene)	63.3	62.9	74.9	62.4	61.2	41.8
$C_{10}H_8$ (azulene)	63.0	57.4	75.2	57.0	56.3	44.4
$CH_3CO_2CH_3$ (Z-methylacetate)	12.6	14.4	21.0	14.4	14.3	8.0
$(CH_3)_3COH$ (t-butanol)	19.9	28.2	27.2	21.9	22.1	13.1
$C_6H_5NH_2$ (aniline)	32.7	32.0	39.1	31.6	31.6	19.8
C_6H_5OH (phenol)	28.6	24.7	35.1	25.2	36.7	14.0
C_4H_6O (divinyl ether)	11.3	10.7	12.9	10.7	10.7	7.2
C_4H_8O (tetrahydrofuran)	16.5	18.0	25.5	18.3	17.8	10.6
C_5H_8O (cyclopentanone)	28.6	28.6	35.6	28.6	28.1	15.7
$C_6H_4O_2$ (benzoquinone)	19.1	36.1	44.6	36.7	35.8	20.9
$C_6H_4N_2$ (pyrimidine)	13.4	12.5	18.4	15.7	15.4	9.0
$(CH_3)_2SO_2$	13.9	12.6	16.7	12.7	12.6	9.5
C_6H_5Cl (chlorobenzene)	24.1	23.7	29.7	23.3	23.6	13.3
$NC(CH_2)_2CN$ (succinonitrile)	15.4	15.2	18.2	15.0	14.7	8.1
$C_4H_4N_2$ (pyrazine)	11.6	11.1	17.4	11.5	10.9	6.4
C_4H_4O (3-butyn-2-one)	11.6	10.1	12.9	10.5	9.7	6.2
C_4H_6O (E-crotonaldehyde)	13.9	15.2	18.7	15.1	15.1	12.6
$C_4H_6O_3$ (acetic anhydride)	21.4	21.3	26.9	21.1	21.1	12.2
C_4H_6S (2,5-dihydrothiophene)	13.3	14.0	17.3	14.1	15.1	7.8
$(CH_3)_2CHCN$	15.0	16.2	22.7	14.5	14.3	9.1
C_4H_8O (methyl ethyl ketone)	17.5	16.0	26.0	20.6	20.1	11.1
$(CH_3)_2CHCHO$	21.5	19.3	26.2	21.4	21.3	11.6
$C_4H_8O_2$ (1,4-dioxane)	19.4	18.4	30.0	21.6	18.1	12.6
C_4H_8S (tetrahydrothiophene)	18.6	16.9	23.9	19.5	18.9	12.9
$(CH_3)_3CCl$	22.7	18.7	26.7	21.6	21.1	13.3
C_4H_9Cl (n-butyl chloride)	17.5	16.6	22.8	19.1	18.4	10.5
C_4H_9N (tetrahydropyrrole)	21.1	21.0	26.7	21.5	20.9	11.8
$C_4H_9NO_2$ (2-nitrobutane)	36.1	36.1	48.4	35.9	35.7	24.9
$(CH_3CH_2)_2O$	16.8	16.6	24.0	20.0	19.2	11.1
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	25.9	24.7	40.1	31.1	30.9	17.7
$(CH_3)_3CSH$	25.4	24.5	37.6	30.2	29.7	17.0
$C_4H_{10}S_2$ (diethyl disulfide)	21.6	18.8	26.6	22.0	21.1	12.8
$(CH_3)_3CNH_2$	23.1	22.7	33.0	26.1	25.9	14.5
$(CH_3)_4Si$	26.7	20.4	28.7	22.8	22.9	13.0
C_5H_6S (2-methyl thiophene)	21.8	21.4	27.9	21.1	21.6	12.0
C_5H_7N (N-methyl pyrrole)	23.7	22.9	28.1	23.3	22.9	13.2
$C_5H_{10}O$ (tetrahydropyran)	29.9	29.6	35.5	29.3	32.8	16.5

(continued)

$(CH_3CH_2)_2C{=}O$	23.2	22.4	28.0	22.4	22.2	16.4
$C_5H_{10}O_2$ (isopropyl acetate)	37.9	35.5	42.6	35.8	35.4	20.5
$C_5H_{10}S$ (tetrahydrothiopyran)	33.8	26.8	36.0	31.3	29.9	17.5
$C_5H_{11}N$ (piperidine)	34.2	32.8	40.2	34.6	33.4	18.8
$C_5H_{12}O$ (t-butyl methyl ether)	33.9	42.0	50.9	41.6	42.0	24.8
$C_6H_4F_2$ (1,3-difluorobenzene)	24.4	22.7	28.1	25.0	22.7	13.3
$C_6H_4F_2$ (1,4-difluorobenzene)	19.0	24.2	23.4	18.3	21.8	11.6
C_6H_5F (fluorobenzene)	23.1	21.8	28.2	21.5	21.2	12.3
$C_6H_{14}O$ (diisopropyl ether)	43.0	54.5	65.2	54.7	54.2	31.2
PF_5	6.5	6.1	7.8	9.9	6.4	3.7
SF_6	6.4	5.8	8.8	6.7	6.5	3.8
P_4	5.0	2.9	4.0	3.3	3.6	2.7
SO_3	3.6	2.1	4.1	2.5	2.3	1.5
SCl_2	4.1	2.6	3.2	3.4	2.9	1.5
$POCl_3$	8.9	7.8	9.9	7.6	7.5	4.4
PCl_5	12.1	8.4	11.2	9.4	8.4	6.3
Cl_2O_2S	7.1	6.3	9.6	6.7	6.4	3.7
PCl_3	4.5	4.0	5.7	4.5	4.5	2.6
Cl_2S_2	4.4	4.3	5.1	4.1	3.9	2.4
$SiCl_2$ ($^1A_1$)	3.0	2.6	3.8	4.5	2.3	2.1
CF_3Cl	5.4	4.4	6.2	4.8	4.4	2.6
C_2F_6	10.3	8.4	10.5	8.7	8.4	4.8
$^2CF_3$	4.1	3.4	4.6	3.4	3.4	2.2
$^2C_6H_5$ (phenyl radical)	35.0	32.2	39.2	29.7	30.1	14.8
Total time	2432.00	2410.90	3036.90	2433.60	2373.70	1417.70
Average time	10.91	10.81	13.62	10.91	10.64	6.36

TABLE IX: Number of SCF cycles required for computing each of the molecules in the G3X/99 test set.

Molecule	r^{2}SCAN	r^{2}SCAN-L				PBE
		PC$_{opt}$	RPP	SRPP	SRPP2	
LiH	7	6	7	6	6	6
^{2}BeH	7	7	7	10	7	7
^{2}CH	7	8	8	7	7	6
CH_2 ($^3B_1$)	7	7	7	7	7	7
CH_2 ($^1A_1$)	6	6	7	6	6	6
$^3CH_3$	6	7	7	6	6	6
CH_4	5	6	7	5	5	6
^{3}NH	7	7	8	7	7	6
NH_2 ($^2B_1$)	7	7	8	7	7	6
NH_3	6	6	7	6	6	6
^{2}OH	7	7	8	7	7	7
H_2O	6	6	6	6	6	6
HF	6	6	7	6	6	6
SiH_2 ($^1A_1$)	6	6	7	6	6	7
SiH_2 ($^3B_1$)	7	8	7	7	7	7
$^2SiH_3$	6	7	6	6	6	6
SiH_4	6	5	6	6	6	6
$^2PH_2$	7	7	7	6	6	6
PH_3	7	6	7	7	7	7
H_2S	7	7	7	7	7	7
HCl	6	7	7	7	7	7
Li_2	5	5	6	5	6	6
LiF	6	7	7	7	7	7
HC≡CH	6	6	7	6	6	6
$H_2C{=}CH_2$	6	6	7	6	6	6
$H_3C{-}CH_3$	6	6	7	6	6	6
CN	12	11	11	11	11	10
HCN	7	7	8	7	7	7
CO	6	7	7	6	6	7
^{2}HCO	8	8	8	8	8	7
H_2CO	7	8	9	7	7	7
CH_3OH	7	8	9	7	7	8
N_2	5	5	5	5	5	5
H_2NNH_2	7	7	7	7	7	7
NO	7	7	7	7	7	12
$^3O_2$	7	7	6	7	7	6
H_2O_2	7	7	7	7	7	7
F_2	6	6	6	6	6	6
CO_2	6	7	6	6	6	7
Na_2	5	6	6	6	6	6
Si_2	8	13	12	12	12	12
P_2	6	6	10	10	10	9
$^3S_2$	7	7	10	7	7	7
Cl_2	6	6	6	7	7	7
NaCl	7	8	9	9	9	9
SiO	7	7	10	9	9	7
CS	7	7	8	8	8	10
SO	8	10	10	10	10	10
ClO	10	10	10	10	16	16

(continued)

ClF	8	8	8	9	9	9
Si_2H_6	6	6	7	7	7	6
CH_3Cl	7	7	7	7	7	7
H_3C-SH	7	7	8	7	7	8
HOCl	7	8	7	8	8	8
SO_2	7	7	7	7	7	7
BF_3	6	6	6	6	6	7
BCl_3	7	8	7	7	7	7
AlF_3	6	6	6	6	6	7
$AlCl_3$	7	6	7	8	8	8
CF_4	6	6	6	6	6	7
CCl_4	8	6	7	8	8	8
OCS	9	9	9	9	9	11
CS_2	7	7	7	7	7	8
F_2CO	8	8	8	8	8	8
SiF_4	6	6	6	6	6	7
$SiCl_4$	7	8	7	7	7	8
NNO	9	8	8	10	10	10
ClNO	27	29	29	28	28	27
NF_3	7	7	7	7	7	7
PF_3	7	6	7	7	7	7
O_3	8	10	9	10	10	7
F_2O	7	7	7	7	7	8
ClF_3	10	11	10	10	19	19
$F_2C=CF_2$	7	7	7	7	7	7
$Cl_2C=CCl_2$	8	8	8	8	8	8
F_3C-CN	10	11	11	11	11	11
$HC\equiv C-CH_3$	7	8	9	8	8	8
$H_2C=C=CH_2$	7	7	8	7	7	7
C_3H_4 (cyclopropene)	7	7	8	7	7	7
$H_2C=CH-CH_3$	7	7	8	7	7	7
C_3H_6 (cyclopropane)	6	6	7	6	6	6
$CH_3-CH_2-CH_3$	7	6	7	7	7	7
C_4H_6 (Z-1,3-butadiene)	7	7	8	8	8	7
C_4H_6 (2-butyne)	7	8	9	7	7	7
C_4H_6 (methylenecyclopropane)	7	7	8	8	8	7
C_4H_6 (bicyclo[1.1.0]butane)	7	7	8	7	7	7
C_4H_6 (cyclobutene)	6	6	8	7	7	7
C_4H_8 (cyclobutane)	6	6	7	7	7	7
C_4H_8 (isobutene)	7	7	8	7	7	8
C_4H_{10} (trans butane)	7	7	8	7	7	7
C_4H_{10} (isobutane)	7	7	8	7	7	7
C_5H_8 (spiropentane)	7	7	7	7	7	7
C_6H_6 (benzene)	8	9	8	8	9	8
CH_2F_2	7	7	9	7	7	7
CHF_3	7	7	9	7	7	7
CH_2Cl_2	7	7	7	7	7	7
$CHCl_3$	8	7	7	8	8	8
CH_3NH_2	7	7	8	7	7	8
CH_3CN	7	9	8	8	8	9
CH_3NO_2 (nitromethane)	10	11	11	11	11	11
CH_3ONO (methyl nitrite)	8	10	10	10	10	10

(continued)

CH_3SiH_3	7	6	7	7	7	7
HCO_2H	9	9	9	9	9	9
HCO_2CH_3	8	8	10	8	8	8
CH_3CONH_2	10	10	10	10	10	10
C_2H_5N (aziridine)	7	8	8	8	8	8
NCCN (cyanogen)	7	7	7	7	7	7
$NH(CH_3)_2$	7	8	8	8	8	8
$CH_3CH_2NH_2$	7	7	8	7	7	8
$H_2C{=}C{=}O$ (ketene)	10	10	10	10	10	10
C_2H_4O (oxirane)	7	8	9	7	7	7
CH_3CHO	9	9	9	9	9	10
$O{=}CH{-}CH{=}O$	7	7	9	7	7	7
CH_3CH_2OH	7	7	9	7	7	8
$(CH_3)_2O$	7	7	9	7	7	7
C_2H_4S (thiooxirane)	8	8	8	8	8	8
$(CH_3)_2S{=}O$	10	10	10	10	10	10
CH_3CH_2SH	7	7	8	8	8	8
$(CH_3)_2S$	7	7	7	7	7	7
$H_2C{=}CHF$	8	8	8	9	9	10
CH_3CH_2Cl	7	7	9	8	8	8
$H_2C{=}CHCl$	8	9	8	8	8	9
$H_2C{=}CHCN$	10	9	10	10	10	11
$(CH_3)_2C{=}O$	7	7	9	8	8	8
CH_3CO_2H	10	10	10	10	10	10
CH_3CFO	8	10	10	10	10	10
CH_3COCl	10	10	10	10	10	11
$CH_3CH_2CH_2Cl$	7	7	8	8	8	8
$(CH_3)_2CHOH$	7	8	8	8	8	8
$CH_3{-}O{-}CH_2CH_3$	7	7	9	8	8	8
$(CH_3)_3N$	7	8	8	8	8	8
C_4H_4O (furan)	8	8	8	8	8	10
C_4H_4S (thiophene)	8	10	8	8	8	10
C_4H_5N (pyrrole)	8	10	10	10	10	10
C_5H_5N (pyridine)	10	10	10	10	10	10
H_2	4	5	5	4	4	5
^2SH	7	7	7	7	7	8
$^2C{\equiv}CH$	15	16	16	15	15	12
$HC{=}CH_2$ ($^2A''$)'	11	11	10	10	10	8
$CH_3C{=}O$ ($^2A''$)'	10	10	10	10	10	10
$CH_2{-}OH$ (^2A)	8	8	8	8	8	8
CH_3O ($^2A''$)'	8	8	9	8	8	13
CH_3CH_2O ($^2A''''$)'	8	8	10	16	16	17
CH_3S ($^2A''$)'	7	8	8	9	9	9
CH_2CH_3 ($^2A''$)'	7	7	8	7	7	7
$(CH_3)_2CH$ ($^2A''$)'	8	8	8	8	8	7
$^2C(CH_3)_3$	8	8	8	8	8	8
NO_2 ($^2A_1$)	7	7	7	7	7	7
$CH_3CH{=}C{=}CH_2$	10	10	10	10	10	10
C_5H_8 (isoprene)	10	10	10	10	10	10
C_5H_{10} (cyclopentane twist)	6	6	7	7	7	7
C_5H_{12} (n-pentane)	7	6	8	7	7	8
$C(CH_3)_4$ (neopentane)	7	8	8	7	7	7

(continued)

C_6H_8 (1,3-cyclohexadiene)	7	8	8	8	8	8
C_6H_8 (1,4-cyclohexadiene)	7	8	8	8	8	8
C_6H_{12} (cyclohexane chair)	7	7	7	7	7	7
C_6H_{14} (n-hexane)	7	6	8	8	8	8
C_6H_{14} (3-methylpentane)	7	8	8	8	8	8
$C_6H_5-CH_3$ (toluene)	8	10	10	10	10	10
C_7H_{16} (n-heptane)	8	8	8	8	8	8
C_8H_8 (cyclooctatetraene)	14	16	8	8	8	8
C_8H_{18} (n-octane)	8	8	8	8	8	8
$C_{10}H_8$ (naphtalene)	10	10	10	10	10	10
$C_{10}H_8$ (azulene)	12	11	12	11	11	14
$CH_3CO_2CH_3$ (Z-methylacetate)	8	10	10	10	10	10
$(CH_3)_3COH$ (t-butanol)	7	10	8	8	8	8
$C_6H_5NH_2$ (aniline)	10	10	10	10	10	10
C_6H_5OH (phenol)	11	10	10	10	15	10
C_4H_6O (divinyl ether)	8	8	8	8	8	10
C_4H_8O (tetrahydrofuran)	7	8	9	8	8	8
C_5H_8O (cyclopentanone)	10	10	10	10	10	10
$C_6H_4O_2$ (benzoquinone)	8	15	15	15	15	15
$C_6H_4N_2$ (pyrimidine)	8	8	10	10	10	10
$(CH_3)_2SO_2$	8	8	8	8	8	10
C_6H_5Cl (chlorobenzene)	10	10	10	10	10	10
$NC(CH_2)_2CN$ (succinonitrile)	10	10	10	10	10	10
$C_4H_4N_2$ (pyrazine)	7	7	9	7	7	7
C_4H_4O (3-butyn-2-one)	10	10	10	10	10	11
C_4H_6O (E-crotonaldehyde)	10	11	10	11	11	16
$C_4H_6O_3$ (acetic anhydride)	10	10	10	10	10	10
C_4H_6S (2,5-dihydrothiophene)	7	8	8	8	8	8
$(CH_3)_2CHCN$	8	9	9	8	8	9
C_4H_8O (methyl ethyl ketone)	8	8	10	10	10	10
$(CH_3)_2CHCHO$	10	9	10	10	10	10
$C_4H_8O_2$ (1,4-dioxane)	7	7	9	8	7	8
C_4H_8S (tetrahydrothiophene)	7	7	8	8	8	8
$(CH_3)_3CCl$	8	7	8	8	8	8
C_4H_9Cl (n-butyl chloride)	7	7	8	8	8	8
C_4H_9N (tetrahydropyrrole)	8	8	8	8	8	8
$C_4H_9NO_2$ (2-nitrobutane)	10	10	11	10	10	11
$(CH_3CH_2)_2O$	7	7	8	8	8	8
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	8	8	10	10	10	10
$(CH_3)_3CSH$	8	8	10	10	10	10
$C_4H_{10}S_2$ (diethyl disulfide)	8	7	8	8	8	8
$(CH_3)_3CNH_2$	7	7	8	8	8	8
$(CH_3)_4Si$	8	6	7	7	7	7
C_5H_6S (2-methyl thiophene)	10	10	10	10	10	10
C_5H_7N (N-methyl pyrrole)	10	10	10	10	10	10
$C_5H_{10}O$ (tetrahydropyran)	8	8	8	8	9	8
$(CH_3CH_2)_2C=O$	8	8	8	8	8	10
$C_5H_{10}O_2$ (isopropyl acetate)	10	10	10	10	10	10
$C_5H_{10}S$ (tetrahydrothiopyran)	8	7	8	8	8	8
$C_5H_{11}N$ (piperidine)	8	8	8	8	8	8
$C_5H_{12}O$ (t-butyl methyl ether)	8	10	10	10	10	10
$C_6H_4F_2$ (1,3-difluorobenzene)	10	10	10	10	10	10

(continued)

$C_6H_4F_2$ (1,4-difluorobenzene)	8	11	8	8	10	9
C_6H_5F (fluorobenzene)	10	10	10	10	10	10
$C_6H_{14}O$ (diisopropyl ether)	8	10	10	10	10	10
PF_5	8	8	8	8	8	8
SF_6	6	6	7	7	7	7
P_4	6	6	6	6	6	7
SO_3	6	6	7	7	7	7
SCl_2	8	9	9	9	9	9
$POCl_3$	10	11	11	11	11	11
PCl_5	10	8	8	8	8	10
Cl_2O_2S	10	10	10	10	10	10
PCl_3	8	9	9	9	9	10
Cl_2S_2	10	10	10	10	10	10
$SiCl_2$ ($^1A_1$)	8	9	8	8	8	9
CF_3Cl	8	8	8	8	8	8
C_2F_6	7	7	7	7	7	7
$^2CF_3$	7	8	7	7	7	7
$^2C_6H_5$ (phenyl radical)	12	11	10	10	10	10
Number of total SCF cycles	1737	1799	1877	1826	1847	1885
Average number SCF cycles	7.79	8.07	8.42	8.19	8.28	8.45
Spread	23	24	24	24	24	22

IV. TIMES IN MOLECULES AND SOLIDS CALCULATED IN VASP-5.4.4

Here we provide the total time and the number of SCF cycles for each molecule from the G3X/99 test set calculated with r^{2}SCAN-L(SRPP) compared r^{2}SCAN-L(RPP), and r^{2}SCAN. Additionally the time and number calculated for solids are reported with different functionals. Calculations from this section were performed with VASP-5.4.4.

TABLE X: Timing in seconds required for computing each of the molecules in the G3X/99 test set in VASP-5.4.4.

Molecule	r^{2}SCAN	r^{2}SCAN-L	
		RPP	SRPP
LiH	30.377	37.216	36.615
^{2}BeH	46.553	101.792	68.080
^{2}CH	46.857	62.547	64.573
CH_2 ($^3B_1$)	52.443	60.135	53.709
CH_2 ($^1A_1$)	29.479	32.485	27.393
$^3CH_3$	60.024	75.065	81.645
CH_4	39.004	26.564	30.968
^{3}NH	55.723	45.079	39.062
NH_2 ($^2B_1$)	58.483	80.918	78.892
NH_3	29.169	33.504	30.359
^{2}OH	49.694	51.292	59.100
H_2O	33.257	17.274	17.328
HF	26.779	16.149	13.195
SiH_2 ($^1A_1$)	27.263	36.056	37.054
SiH_2 ($^3B_1$)	55.402	118.375	94.207
$^2SiH_3$	61.082	342.021	163.892
SiH_4	43.306	47.260	58.662
$^2PH_2$	55.311	131.165	125.100
PH_3	26.204	46.563	51.389
H_2S	27.166	43.727	40.557
HCl	24.483	27.308	20.656
Li_2	23.147	44.294	37.898
LiF	47.112	15.760	18.413
HC≡CH	35.163	16.601	20.589
$H_2C{=}CH_2$	38.735	24.968	25.066
$H_3C{-}CH_3$	46.479	38.170	44.965
CN	65.863	101.853	121.749
HCN	34.307	27.922	26.719
CO	29.189	26.025	20.412
^{2}HCO	60.956	158.008	134.285
H_2CO	34.094	36.690	25.367
CH_3OH	47.071	29.334	34.200
N_2	26.080	35.479	41.829
H_2NNH_2	39.501	46.185	36.926
NO	57.008	64.290	139.923
$^3O_2$	49.309	81.066	80.426
H_2O_2	26.402	33.140	21.234
F_2	25.739	11.958	11.771
CO_2	33.984	24.252	22.650
Na_2	21.433	56.720	41.140
Si_2	51.941	121.550	97.707
P_2	24.910	26.306	74.310
$^3S_2$	49.552	159.375	93.464

(continued)

Cl_2	27.404	31.285	19.328
NaCl	40.057	28.024	27.936
SiO	38.603	26.843	16.398
CS	26.686	33.624	34.545
SO	58.042	98.033	136.573
ClO	58.870	171.075	113.411
ClF	28.886	20.161	15.332
Si_2H_6	52.189	66.321	125.253
CH_3Cl	42.664	42.031	34.189
H_3C-SH	48.304	56.916	56.903
HOCl	31.965	31.090	19.747
SO_2	38.238	40.939	25.698
BF_3	37.197	30.890	16.120
BCl_3	38.547	48.497	47.192
AlF_3	44.881	25.294	23.337
$AlCl_3$	39.541	59.578	49.828
CF_4	44.732	27.426	22.547
CCl_4	37.877	56.132	57.452
OCS	33.083	33.738	26.176
CS_2	30.524	39.271	40.038
F_2CO	38.397	21.691	19.096
SiF_4	56.522	40.358	27.121
$SiCl_4$	51.793	62.520	57.635
NNO	33.232	35.228	34.646
ClNO	35.928	33.513	28.091
NF_3	30.336	23.603	18.999
PF_3	30.514	36.110	23.427
O_3	33.462	30.513	26.833
F_2O	31.782	17.559	17.333
ClF_3	38.878	26.870	18.577
$F_2C=CF_2$	41.589	26.282	22.340
$Cl_2C=CCl_2$	42.696	45.655	47.673
F_3C-CN	63.184	52.305	63.820
$HC\equiv C-CH_3$	52.260	32.313	37.241
$H_2C=C=CH_2$	49.648	31.769	32.724
C_3H_4 (cyclopropene)	54.086	42.388	38.496
$H_2C=CH-CH_3$	56.039	45.608	41.997
C_3H_6 (cyclopropane)	40.705	41.351	39.021
$CH_3-CH_2-CH_3$	43.352	42.736	52.029
C_4H_6 (Z-1,3-butadiene)	51.881	47.408	37.217
C_4H_6 (2-butyne)	53.967	43.340	41.759
C_4H_6 (methylenecyclopropane)	56.056	45.149	43.333
C_4H_6 (bicyclo[1.1.0]butane)	49.732	46.964	45.781
C_4H_6 (cyclobutene)	54.769	42.438	42.824
C_4H_8 (cyclobutane)	44.921	44.999	53.150
C_4H_8 (isobutene)	61.122	48.967	60.395
C_4H_{10} (trans butane)	62.071	53.963	60.280
C_4H_{10} (isobutane)	51.161	48.957	60.090
C_5H_8 (spiropentane)	48.760	51.205	57.503
C_6H_6 (benzene)	56.865	64.889	42.343
CH_2F_2	37.226	34.515	20.908
CHF_3	28.350	30.801	18.654

(continued)

CH_2Cl_2	44.070	61.817	36.144
$CHCl_3$	43.822	57.695	52.874
CH_3NH_2	35.850	37.467	35.972
CH_3CN	39.086	41.409	56.041
CH_3NO_2 (nitromethane)	37.919	45.303	38.357
CH_3ONO (methyl nitrite)	52.397	53.712	40.054
CH_3SiH_3	56.856	52.314	65.291
HCO_2H	37.162	34.614	26.941
HCO_2CH_3	44.830	52.762	41.339
CH_3CONH_2	42.642	44.315	51.743
C_2H_5N (aziridine)	45.664	49.546	44.309
NCCN (cyanogen)	32.373	51.770	36.523
$NH(CH_3)_2$	42.250	43.500	53.879
$CH_3CH_2NH_2$	47.554	51.101	62.002
$H_2C{=}C{=}O$ (ketene)	41.942	34.368	26.212
C_2H_4O (oxirane)	48.431	39.788	34.471
CH_3CHO	35.358	41.606	35.985
$O{=}CH{-}CH{=}O$	42.393	41.016	32.879
CH_3CH_2OH	56.036	45.612	44.639
$(CH_3)_2O$	54.735	44.090	42.475
C_2H_4S (thiooxirane)	46.398	54.440	50.330
$(CH_3)_2S{=}O$	49.164	40.358	60.584
CH_3CH_2SH	51.562	57.135	59.840
$(CH_3)_2S$	53.493	50.524	56.638
$H_2C{=}CHF$	44.478	28.691	26.361
CH_3CH_2Cl	37.864	39.836	38.422
$H_2C{=}CHCl$	39.015	39.007	29.574
$H_2C{=}CHCN$	44.296	43.039	51.750
$(CH_3)_2C{=}O$	44.507	38.441	45.737
CH_3CO_2H	54.873	52.693	40.032
CH_3CFO	41.480	30.644	32.793
CH_3COCl	51.734	53.154	40.173
$CH_3CH_2CH_2Cl$	53.445	48.507	60.796
$(CH_3)_2CHOH$	51.395	48.865	58.707
$CH_3{-}O{-}CH_2CH_3$	64.466	53.694	49.400
$(CH_3)_3N$	51.278	51.033	59.060
C_4H_4O (furan)	50.525	45.000	31.626
C_4H_4S (thiophene)	51.251	51.357	40.410
C_4H_5N (pyrrole)	55.006	46.450	38.781
C_5H_5N (pyridine)	54.926	53.125	44.318
H_2	25.091	16.790	10.425
^2SH	51.139	118.354	237.039
$^2C{\equiv}CH$	84.452	237.466	136.243
'$HC{=}CH_2$ ($^2A''$)'	76.701	230.745	154.313
'$CH_3C{=}O$ ($^2A''$)'	76.421	154.706	176.016
$CH_2{-}OH$ (^2A)	52.205	149.264	115.682
'CH_3O ($^2A''$)'	46.004	95.070	109.511
'CH_3CH_2O ($^2A''''$)'	74.700	180.107	169.691
'CH_3S ($^2A''$)'	73.964	160.302	165.232
'CH_2CH_3 ($^2A''$)'	73.505	118.128	101.164
'$(CH_3)_2CH$ ($^2A''$)'	65.068	175.942	139.259
$^2C(CH_3)_3$	82.072	316.997	257.057

(continued)

NO_2 ($^2A_1$)	57.303	101.336	151.466
$CH_3CH{=}C{=}CH_2$	52.813	51.393	44.123
C_5H_8 (isoprene)	58.762	54.955	49.219
C_5H_{10} (cyclopentane twist)	46.451	51.819	62.560
C_5H_{12} (n-pentane)	62.483	61.589	67.535
$C(CH_3)_4$ (neopentane)	69.363	60.296	70.803
C_6H_8 (1,3-cyclohexadiene)	73.235	64.774	64.059
C_6H_8 (1,4-cyclohexadiene)	60.395	57.682	53.948
C_6H_{12} (cyclohexane chair)	50.209	61.903	71.651
C_6H_{14} (n-hexane)	70.945	68.738	80.399
C_6H_{14} (3-methylpentane)	71.994	68.097	85.687
$C_6H_5{-}CH_3$ (toluene)	62.408	68.435	66.284
C_7H_{16} (n-heptane)	90.709	76.170	89.036
C_8H_8 (cyclooctatetraene)	60.808	59.398	48.524
C_8H_{18} (n-octane)	103.047	98.131	117.752
$C_{10}H_8$ (naphtalene)	75.862	66.975	54.421
$C_{10}H_8$ (azulene)	71.855	80.485	76.085
$CH_3CO_2CH_3$ (Z-methylacetate)	56.501	55.723	47.641
$(CH_3)_3COH$ (t-butanol)	67.541	48.672	67.334
$C_6H_5NH_2$ (aniline)	59.786	64.089	52.127
C_6H_5OH (phenol)	52.683	61.007	43.772
C_4H_6O (divinyl ether)	52.519	47.567	38.660
C_4H_8O (tetrahydrofuran)	57.301	58.500	63.350
C_5H_8O (cyclopentanone)	50.249	58.541	69.151
$C_6H_4O_2$ (benzoquinone)	50.111	59.858	47.191
$C_6H_4N_2$ (pyrimidine)	50.956	53.440	54.258
$(CH_3)_2SO_2$	60.469	44.040	64.055
C_6H_5Cl (chlorobenzene)	50.184	68.510	47.653
$NC(CH_2)_2CN$ (succinonitrile)	54.590	56.337	74.380
$C_4H_4N_2$ (pyrazine)	42.943	43.521	48.426
C_4H_4O (3-butyn-2-one)	42.471	50.552	44.816
C_4H_6O (E-crotonaldehyde)	58.628	63.398	60.674
$C_4H_6O_3$ (acetic anhydride)	53.349	67.071	71.050
C_4H_6S (2,5-dihydrothiophene)	49.174	52.918	47.245
$(CH_3)_2CHCN$	67.867	64.799	76.422
C_4H_8O (methyl ethyl ketone)	45.440	47.696	57.552
$(CH_3)_2CHCHO$	69.392	68.922	72.834
$C_4H_8O_2$ (1,4-dioxane)	60.810	65.409	66.824
C_4H_8S (tetrahydrothiophene)	58.441	60.940	71.827
$(CH_3)_3CCl$	63.884	71.304	71.030
C_4H_9Cl (n-butyl chloride)	56.282	58.558	68.254
C_4H_9N (tetrahydropyrrole)	55.330	53.245	61.243
$C_4H_9NO_2$ (2-nitrobutane)	53.425	62.385	70.275
$(CH_3CH_2)_2O$	66.875	60.805	73.004
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	74.373	68.726	81.966
$(CH_3)_3CSH$	47.861	57.674	73.993
$C_4H_{10}S_2$ (diethyl disulfide)	52.868	86.959	86.515
$(CH_3)_3CNH_2$	48.920	56.591	74.385
$(CH_3)_4Si$	52.672	67.158	72.778
C_5H_6S (2-methyl thiophene)	55.038	62.434	66.285
C_5H_7N (N-methyl pyrrole)	44.628	48.375	47.003
$C_5H_{10}O$ (tetrahydropyran)	66.396	56.566	73.107

(continued)

$(CH_3CH_2)_2C{=}O$	65.943	55.250	66.029
$C_5H_{10}O_2$ (isopropyl acetate)	54.201	51.654	77.247
$C_5H_{10}S$ (tetrahydrothiopyran)	58.347	61.648	71.019
$C_5H_{11}N$ (piperidine)	66.287	65.947	77.307
$C_5H_{12}O$ (t-butyl methyl ether)	77.209	63.770	80.962
$C_6H_4F_2$ (1,3-difluorobenzene)	51.266	48.566	39.639
$C_6H_4F_2$ (1,4-difluorobenzene)	50.014	48.794	35.479
C_6H_5F (fluorobenzene)	58.243	54.627	43.368
$C_6H_{14}O$ (diisopropyl ether)	80.435	67.774	88.576
PF_5	53.031	48.204	27.992
SF_6	69.459	42.138	28.931
P_4	36.332	37.723	147.808
SO_3	37.472	37.628	24.160
SCl_2	30.768	40.682	32.715
$POCl_3$	53.473	59.149	57.917
PCl_5	57.929	84.332	62.172
Cl_2O_2S	48.150	49.434	41.294
PCl_3	39.120	58.508	49.139
Cl_2S_2	38.077	61.863	49.617
$SiCl_2$ ($^1A_1$)	30.864	49.387	42.754
CF_3Cl	46.195	47.000	34.081
C_2F_6	52.305	35.433	30.804
$^2CF_3$	72.385	95.930	87.270
$^2C_6H_5$ (phenyl radical)	104.816	408.504	225.183
Total time	11100.38	13573.66	13030.01
Average time	49.78	60.87	58.43

TABLE XI: Number of SCF cycles required required for computing each of the molecules in the G3X/99 test set in VASP-5.4.4.

Molecule	r^{2}SCAN	r^{2}SCAN-L	
		RPP	SRPP
LiH	17	65	53
^{2}BeH	15	82	50
^{2}CH	15	50	47
CH_2 ($^3B_1$)	16	44	36
CH_2 ($^1A_1$)	15	49	35
$^3CH_3$	17	52	52
CH_4	17	33	33
^{3}NH	17	36	29
NH_2 ($^2B_1$)	17	56	50
NH_3	18	48	36
^{2}OH	17	43	45
H_2O	18	27	23
HF	16	29	20
SiH_2 ($^1A_1$)	14	54	47
SiH_2 ($^3B_1$)	16	83	60
$^2SiH_3$	16	176	76
SiH_4	15	47	49
$^2PH_2$	16	91	79
PH_3	15	64	60
H_2S	14	66	52
HCl	14	47	30
Li_2	12	69	49
LiF	26	26	26
HC≡CH	17	24	26
$H_2C{=}CH_2$	17	31	27
$H_3C{-}CH_3$	18	35	35
CN	20	80	86
HCN	16	42	34
CO	16	44	29
^{2}HCO	18	114	88
H_2CO	17	53	31
CH_3OH	18	32	32
N_2	15	61	58
H_2NNH_2	18	50	33
NO	18	51	98
$^3O_2$	16	65	59
H_2O_2	16	46	25
F_2	15	20	17
CO_2	17	36	29
Na_2	11	86	52
Si_2	15	89	65
P_2	14	44	105
$^3S_2$	16	126	68
Cl_2	14	48	25
NaCl	20	42	36
SiO	21	45	23
CS	15	57	49
SO	18	78	98
ClO	18	136	82

(continued)

ClF	16	34	22
Si_2H_6	15	57	91
CH_3Cl	16	46	32
H_3C-SH	16	56	48
HOCl	16	45	24
SO_2	17	52	28
BF_3	17	41	18
BCl_3	15	55	46
AlF_3	18	29	23
$AlCl_3$	15	66	47
CF_4	17	29	21
CCl_4	15	53	46
OCS	16	50	33
CS_2	15	57	49
F_2CO	17	28	21
SiF_4	17	35	20
$SiCl_4$	15	54	42
NNO	16	53	44
ClNO	16	42	30
NF_3	17	31	21
PF_3	17	49	26
O_3	17	45	34
F_2O	16	25	21
ClF_3	17	34	20
$F_2C=CF_2$	16	30	22
$Cl_2C=CCl_2$	16	51	45
F_3C-CN	18	44	46
$HC\equiv C-CH_3$	18	32	31
$H_2C=C=CH_2$	17	33	29
C_3H_4 (cyclopropene)	18	42	32
$H_2C=CH-CH_3$	18	42	33
C_3H_6 (cyclopropane)	18	44	35
$CH_3-CH_2-CH_3$	18	43	44
C_4H_6 (Z-1,3-butadiene)	18	48	32
C_4H_6 (2-butyne)	18	41	35
C_4H_6 (methylenecyclopropane)	18	43	35
C_4H_6 (bicyclo[1.1.0]butane)	19	43	35
C_4H_6 (cyclobutene)	18	41	35
C_4H_8 (cyclobutane)	18	42	42
C_4H_8 (isobutene)	18	42	43
C_4H_{10} (trans butane)	18	46	44
C_4H_{10} (isobutane)	19	43	44
C_5H_8 (spiropentane)	18	46	43
C_6H_6 (benzene)	18	61	33
CH_2F_2	16	43	22
CHF_3	16	41	21
CH_2Cl_2	15	61	30
$CHCl_3$	15	56	44
CH_3NH_2	18	45	36
CH_3CN	17	43	49
CH_3NO_2 (nitromethane)	17	48	34
CH_3ONO (methyl nitrite)	17	51	32

(continued)

CH_3SiH_3	17	46	48
HCO_2H	17	46	30
HCO_2CH_3	17	48	31
CH_3CONH_2	18	43	43
C_2H_5N (aziridine)	18	46	35
NCCN (cyanogen)	16	75	46
$NH(CH_3)_2$	18	43	43
$CH_3CH_2NH_2$	18	46	47
$H_2C{=}C{=}O$ (ketene)	18	43	28
C_2H_4O (oxirane)	18	43	32
CH_3CHO	18	50	36
$O{=}CH{-}CH{=}O$	17	48	32
CH_3CH_2OH	18	43	36
$(CH_3)_2O$	18	42	34
C_2H_4S (thiooxirane)	16	53	42
$(CH_3)_2S{=}O$	18	34	44
CH_3CH_2SH	17	54	48
$(CH_3)_2S$	17	46	44
$H_2C{=}CHF$	18	33	26
CH_3CH_2Cl	17	42	34
$H_2C{=}CHCl$	16	44	29
$H_2C{=}CHCN$	17	47	48
$(CH_3)_2C{=}O$	18	36	36
CH_3CO_2H	18	50	32
CH_3CFO	18	32	29
CH_3COCl	17	52	33
$CH_3CH_2CH_2Cl$	17	44	47
$(CH_3)_2CHOH$	19	42	43
$CH_3{-}O{-}CH_2CH_3$	19	46	36
$(CH_3)_3N$	19	44	43
C_4H_4O (furan)	18	45	27
C_4H_4S (thiophene)	17	48	32
C_4H_5N (pyrrole)	18	44	31
C_5H_5N (pyridine)	18	50	35
H_2	15	32	17
^2SH	16	94	170
$^2C{\equiv}CH$	22	155	79
'$HC{=}CH_2$ ($^2A''$)'	20	144	87
'$CH_3C{=}O$ ($^2A''$)'	18	82	85
$CH_2{-}OH$ (^2A)	18	87	63
'CH_3O ($^2A''$)'	17	61	64
'CH_3CH_2O ($^2A''''$)'	18	78	66
'CH_3S ($^2A''$)'	17	86	79
'CH_2CH_3 ($^2A''$)'	17	63	49
'$(CH_3)_2CH$ ($^2A''$)'	18	89	63
$^2C(CH_3)_3$	18	125	89
NO_2 ($^2A_1$)	17	66	90
$CH_3CH{=}C{=}CH_2$	18	46	33
C_5H_8 (isoprene)	18	45	34
C_5H_{10} (cyclopentane twist)	18	43	43
C_5H_{12} (n-pentane)	18	47	44
$C(CH_3)_4$ (neopentane)	18	47	47

(continued)

C_6H_8 (1,3-cyclohexadiene)	18	43	36
C_6H_8 (1,4-cyclohexadiene)	18	46	36
C_6H_{12} (cyclohexane chair)	18	47	46
C_6H_{14} (n-hexane)	18	45	45
C_6H_{14} (3-methylpentane)	18	44	48
$C_6H_5{-}CH_3$ (toluene)	18	52	43
C_7H_{16} (n-heptane)	18	46	47
C_8H_8 (cyclooctatetraene)	17	46	32
C_8H_{18} (n-octane)	19	47	49
$C_{10}H_8$ (naphtalene)	18	49	34
$C_{10}H_8$ (azulene)	18	53	43
$CH_3CO_2CH_3$ (Z-methylacetate)	18	47	34
$(CH_3)_3COH$ (t-butanol)	19	36	43
$C_6H_5NH_2$ (aniline)	18	51	35
C_6H_5OH (phenol)	18	55	33
C_4H_6O (divinyl ether)	18	43	29
C_4H_8O (tetrahydrofuran)	18	48	44
C_5H_8O (cyclopentanone)	18	45	44
$C_6H_4O_2$ (benzoquinone)	17	53	35
$C_6H_4N_2$ (pyrimidine)	18	50	43
$(CH_3)_2SO_2$	18	34	43
C_6H_5Cl (chlorobenzene)	17	61	36
$NC(CH_2)_2CN$ (succinonitrile)	17	47	53
$C_4H_4N_2$ (pyrazine)	17	45	43
C_4H_4O (3-butyn-2-one)	18	46	34
C_4H_6O (E-crotonaldehyde)	18	52	42
$C_4H_6O_3$ (acetic anhydride)	18	49	43
C_4H_6S (2,5-dihydrothiophene)	17	48	36
$(CH_3)_2CHCN$	18	46	46
C_4H_8O (methyl ethyl ketone)	19	43	44
$(CH_3)_2CHCHO$	19	50	45
$C_4H_8O_2$ (1,4-dioxane)	18	51	44
C_4H_8S (tetrahydrothiophene)	17	47	47
$(CH_3)_3CCl$	18	53	45
C_4H_9Cl (n-butyl chloride)	17	45	47
C_4H_9N (tetrahydropyrrole)	18	46	45
$C_4H_9NO_2$ (2-nitrobutane)	19	47	45
$(CH_3CH_2)_2O$	19	46	47
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	18	44	46
$(CH_3)_3CSH$	18	46	50
$C_4H_{10}S_2$ (diethyl disulfide)	17	60	50
$(CH_3)_3CNH_2$	18	45	50
$(CH_3)_4Si$	17	45	42
C_5H_6S (2-methyl thiophene)	17	51	45
C_5H_7N (N-methyl pyrrole)	18	42	34
$C_5H_{10}O$ (tetrahydropyran)	19	43	48
$(CH_3CH_2)_2C{=}O$	19	42	43
$C_5H_{10}O_2$ (isopropyl acetate)	18	36	46
$C_5H_{10}S$ (tetrahydrothiopyran)	17	47	46
$C_5H_{11}N$ (piperidine)	18	47	47
$C_5H_{12}O$ (t-butyl methyl ether)	19	41	44
$C_6H_4F_2$ (1,3-difluorobenzene)	18	45	31

(continued)

$C_6H_4F_2$ (1,4-difluorobenzene)	18	46	28
C_6H_5F (fluorobenzene)	18	49	33
$C_6H_{14}O$ (diisopropyl ether)	19	42	47
PF_5	17	41	20
SF_6	18	32	19
P_4	15	45	150
SO_3	17	44	24
SCl_2	15	52	35
$POCl_3$	17	50	42
PCl_5	16	64	40
Cl_2O_2S	17	46	33
PCl_3	15	58	42
Cl_2S_2	15	65	44
$SiCl_2$ ($^1A_1$)	15	63	46
CF_3Cl	17	46	28
C_2F_6	17	30	22
$^2CF_3$	18	54	45
$^2C_6H_5$ (phenyl radical)	21	189	95
Number of total SCF cycles	3841	11573	9621
Average number SCF cycles	17.22	51.90	43.14

TABLE XII. Timing in seconds required for computing each of the 55 solids in the solid test set. Computational details can see in the manuscript for the case 0.

Molecule	r^{2}SCAN	r^{2}SCAN-L				PBE
		PC$_{opt}$	RPP	SRPP	SRPP2	
C	33.034	23.962	22.138	19.422	19.662	21.946
Si	65.007	151.698	45.032	38.060	35.971	26.402
Ge	84.081	435.321	324.345	33.284	34.761	31.047
Sn	107.107	90.177	147.412	135.179	155.290	37.773
SiC	44.550	33.235	23.557	23.376	23.849	22.033
BN	39.184	34.500	23.770	21.633	21.550	22.534
BP	47.696	50.314	23.041	23.707	23.272	24.659
AlN	43.149	44.481	26.528	25.374	24.998	23.213
AlP	71.379	199.870	60.160	74.237	132.400	28.642
AlAs	89.168	127.986	92.719	145.653	85.386	32.621
GaN	59.302	43.298	26.764	27.527	26.496	26.527
GaP	76.477	99.710	299.694	42.391	39.150	30.072
GaAs	90.528	172.090	161.612	169.166	153.046	33.664
InP	90.466	250.460	92.541	155.946	198.743	33.825
InAs	92.330	283.677	149.608	122.780	151.050	35.101
InSb	110.318	636.426	179.537	134.863	173.764	40.006
LiH	44.011	34.041	80.493	46.323	36.058	20.917
LiF	41.101	43.625	23.547	22.445	21.472	22.614
LiCl	73.165	39.155	28.741	28.222	28.350	26.648
NaF	48.025	35.479	24.211	25.325	24.175	24.519
NaCl	71.365	131.549	76.282	66.857	66.555	29.492
MgO	45.335	28.381	25.106	26.080	24.647	23.912
Li	39.523	35.433	31.216	31.877	31.516	22.611
Na	60.950	41.204	64.044	47.932	47.827	27.750
K	116.116	101.673	133.850	130.132	120.144	41.752
Rb	201.052	158.444	424.013	139.482	198.437	51.198
Cs	158.715	313.501	775.530	575.539	135.791	57.268
Ca	90.474	48.488	36.580	37.767	36.691	31.657
Ba	103.659	268.256	225.715	112.099	85.427	39.879
Sr	107.558	204.399	53.822	62.741	52.065	37.340
Al	102.044	45.067	29.195	32.409	30.687	25.573
Fe	231.163	250.898	390.057	361.941	333.449	109.842
Co	125.871	134.440	219.715	205.561	274.006	85.227
Ni	122.939	173.167	151.279	159.796	147.358	68.564
Sc	364.658	267.462	152.964	152.001	150.533	144.638
Y	402.284	212.809	180.641	195.709	192.475	149.670
Ti	252.911	199.312	106.910	108.243	106.264	108.297
Zr	251.091	220.845	167.506	177.940	171.898	112.560
Hf	216.780	396.223	109.505	108.757	109.757	96.080
V	61.746	39.647	35.772	33.616	32.522	36.462
Nb	76.495	105.134	38.084	37.827	36.081	37.818
Ta	55.812	33.855	34.747	48.970	47.580	51.054
Mo	80.585	92.472	34.021	34.035	33.016	33.596
W	69.591	39.390	34.101	34.959	34.393	34.186
Tc	205.485	213.185	97.318	101.540	104.510	101.089
Re	284.283	362.795	137.901	145.469	141.327	140.429
Ru	223.500	282.835	101.795	97.903	96.688	102.086
Os	188.606	150.246	97.590	97.211	95.955	94.792
Rh	49.676	62.053	27.450	28.164	27.011	30.151
Ir	59.296	74.898	29.108	31.877	31.921	26.090
Pd	84.709	57.729	29.238	31.707	30.987	27.134
Pt	49.860	50.329	24.495	29.353	28.110	27.502
Cu	41.947	29.123	25.511	26.328	25.425	26.883
Ag	49.431	85.538	40.812	37.590	36.080	25.657
Au	57.226	72.011	27.305	28.080	27.093	27.441
Total time	6052.81	7812.30	6024.63	4892.41	4553.67	2650.44
Average time	110.05	142.04	109.54	88.95	82.79	48.19

TABLE XIII. As in Table XII but for the Number of SCF cycles

Molecule	r^{2}SCAN	r^{2}SCAN-L				PBE
		PC$_{opt}$	RPP	SRPP	SRPP2	
C	12	18	13	11	11	11
Si	12	98	23	19	18	11
Ge	12	265	162	12	12	11
Sn	13	35	63	57	69	12
SiC	13	21	13	13	13	12
BN	14	26	14	13	13	12
BP	13	34	12	12	12	12
AlN	13	39	15	14	14	13
AlP	13	136	33	43	83	12
AlAs	13	72	43	68	41	12
GaN	13	27	13	13	13	13
GaP	13	57	164	18	16	12
GaAs	13	97	79	78	75	12
InP	13	143	41	79	97	12
InAs	13	159	71	61	71	12
InSb	13	355	78	54	75	12
LiH	12	23	62	30	25	11
LiF	12	40	13	12	12	12
LiCl	13	18	13	13	13	12
NaF	13	24	13	14	13	13
NaCl	13	80	43	37	37	13
MgO	12	14	13	13	13	12
Li	10	16	15	15	15	9
Na	10	16	29	20	20	9
K	14	35	49	46	44	12
Rb	19	47	139	49	63	12
Cs	14	97	254	187	149	13
Ca	16	22	16	16	16	13
Ba	14	103	91	42	32	12
Sr	16	112	23	25	22	13
Al	34	45	16	20	19	13
Fe	42	73	102	91	90	27
Co	24	51	81	64	97	26
Ni	21	63	57	49	49	19
Sc	23	44	23	23	23	21
Y	16	24	21	23	23	16
Ti	18	36	17	17	17	17
Zr	16	36	25	29	26	15
Hf	13	71	15	15	15	12
V	17	18	15	15	15	16
Nb	19	52	17	16	16	17
Ta	12	14	14	25	25	28
Mo	20	46	14	13	13	14
W	16	19	15	15	15	15
Tc	15	39	14	15	15	15
Re	22	72	24	25	24	24
Ru	17	55	16	15	15	17
Os	14	31	15	15	15	14
Rh	13	41	13	13	13	19
Ir	16	49	16	16	17	14
Pd	24	42	16	17	17	13
Pt	13	31	13	14	14	13
Cu	14	17	15	15	15	14
Ag	13	72	22	20	20	12
Au	14	47	13	13	13	13
Number of total SCF cycles	860	3317	2219	1677	1728	781
Average number SCF cycles	15.64	60.31	40.35	30.49	31.42	14.20
Spread	32	341	242	176	138	19

V. MOLECULAR DYNAMICS OF ALUMINUM

In this section, we present various plots related to the AIMD calculations on Al described in the main paper. The system is 108 atoms, at bulk density $\rho = 2.34$ g/cm^3 in a $12.7239 \times 12.7239 \times 12.7239$ Å^3 cell. Γ-point sampling was done in the Brillouin zone. In VASP 5.4.4, the calculations used a three-electron pseudopotential ($3s^2\ 3p^1$ valence (10 core electrons; denoted PAW_PBE Al_GW). Non-spherical contributions within the PAW spheres were included self-consistently. Minimization used the RMM-DISS algorithm with energy cutoff set to 500 eV. The self-consistent energy convergence tolerance E_{diff} was 1×10^{-4} eV. Molecular dynamics used the Verlet algorithm and a Nosé thermostat. 6501 steps of time-step 0.941 femtoseconds were taken for each simulation.

Approximate Fermi-type thermal smearing with a width of 0.0881555 eV was used for ion temperature T=1023 K. For T=298 K ion temperature, the smearing width was 0.025680 eV.

Figure 1 shows the behavior of the SCF cycle count over the first 50 steps of the T=1023 K molecular dynamics of aluminum for various XC functionals of interest. This is complementary with the Figure for 100 steps in the main text.

Figure 2 shows the mean-squared displacement as a function of time (MD step) and the radial distribution function for Al at T=1023 K for the XC functionals of interest. Figure 3 gives comparable results for T = 298 K.

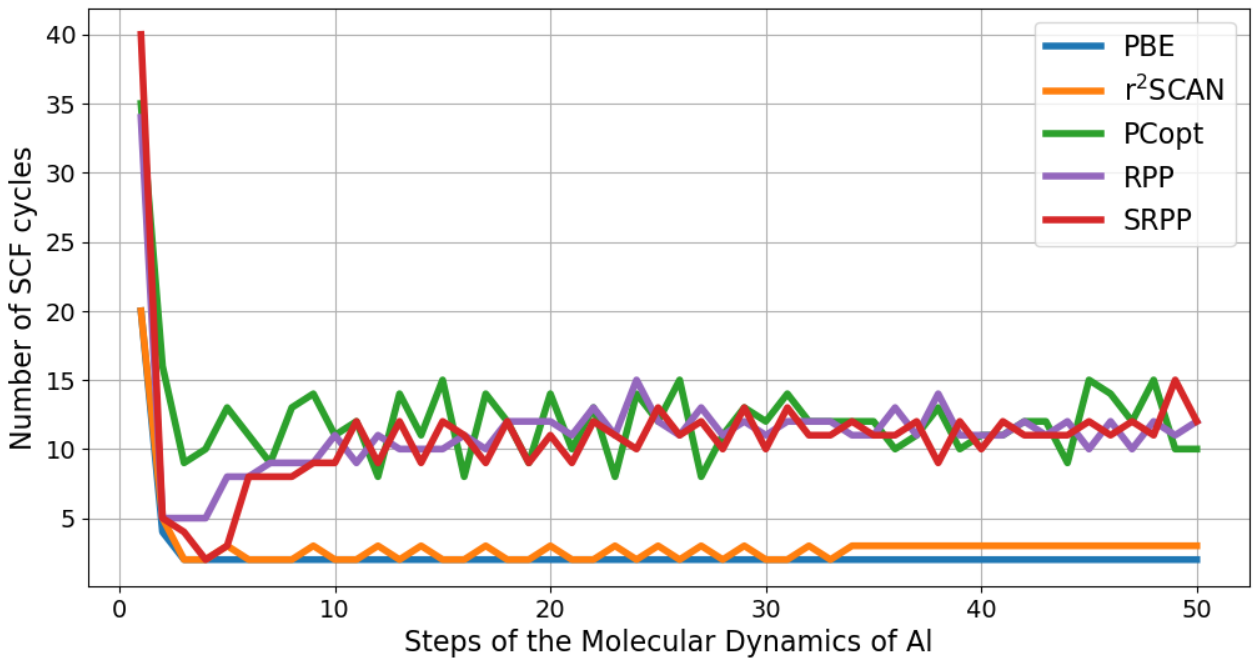


FIG. 1. SCF cycle count behavior over the first 50 steps of the AIMD simulation of Al, $\rho = 2.34$ g/cm^3, T=1023 K for various XC functionals.

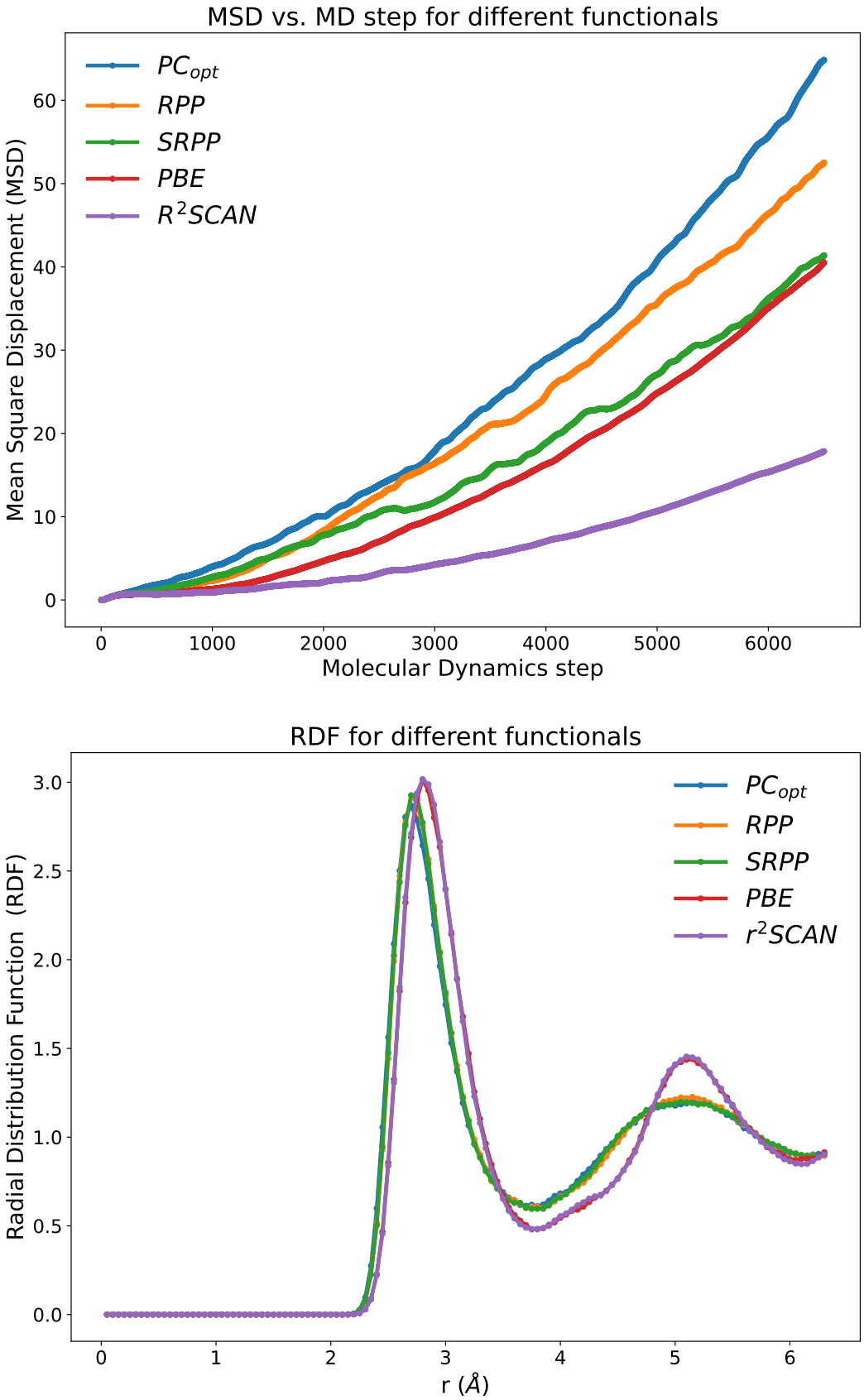
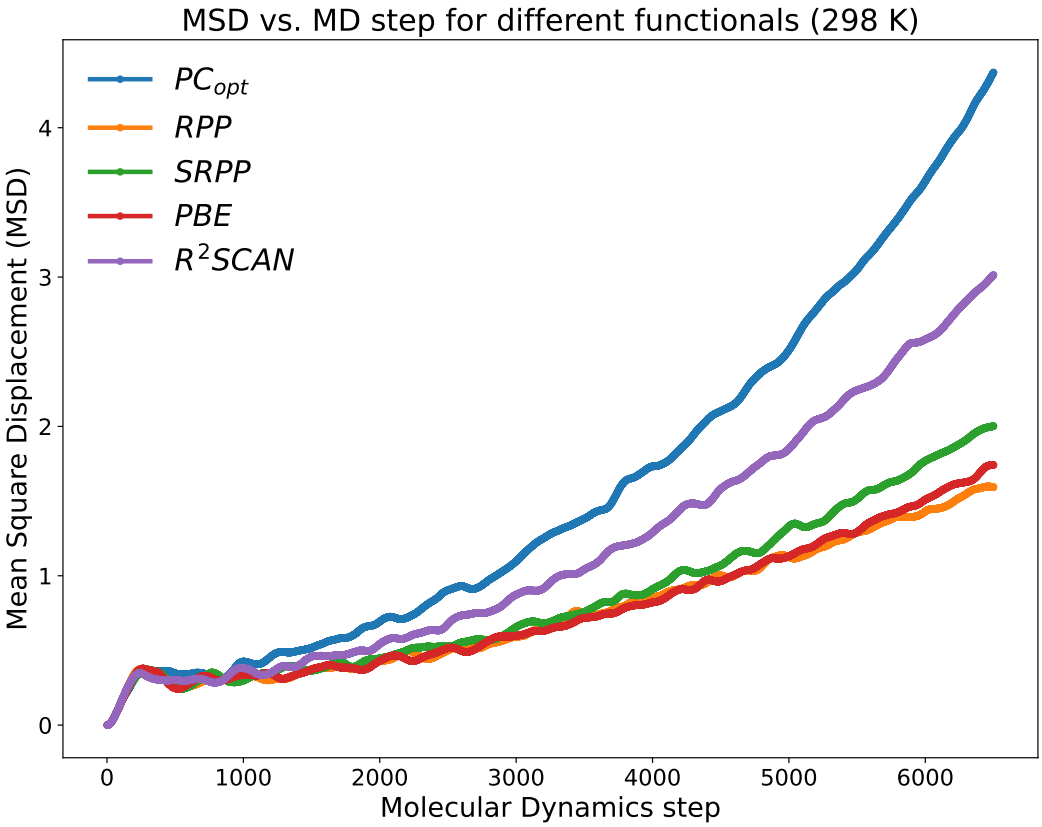


FIG. 2. Mean-squared displacement as a function of MD step and resulting RDF for Al at T =1023 K, $\rho = 2.34$ g/cm^3 from r^{2}SCAN, and r^{2}SCAN-L with the PC$_{\text{opt}}$, RPP, and SRPP deorbitalizers.



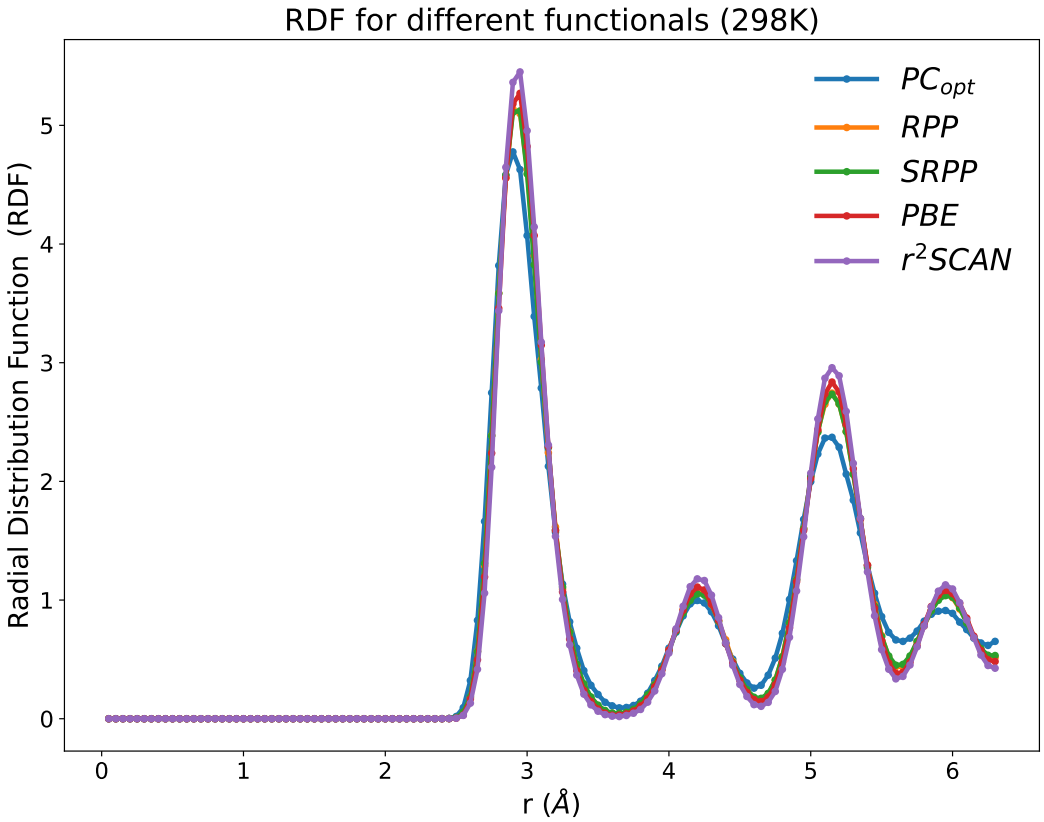


FIG. 3. As in 2 but for T=298 K. Note the different scale for the MSD.

A. Analysis of forces in Molecular Dynamics of Aluminum

Figure 4 displays the maximum, minimum, and median forces in the z direction for the first 50 (top) and 500 (bottom) steps of the molecular dynamics simulation of aluminum. Each step reports 108 forces, one for each ion. For each force component, the maximum, minimum, and median values were extracted for different functionals to identify any possible outliers.

The plots indicate that the behavior of the forces for the deorbitalized functionals does not show any anomalies, as no outliers are observed. The range of forces is comparable to that obtained with PBE and r^{2}SCAN. In all cases, the median values remain consistently close to zero, suggesting that the forces acting on the nuclei are symmetrically distributed around zero and that no systematic bias is introduced by the deorbitalized functionals.

The analysis for 500 steps (bottom) shows the same behavior as observed in the first 50 steps, confirming the stability of the forces over a longer simulation period.

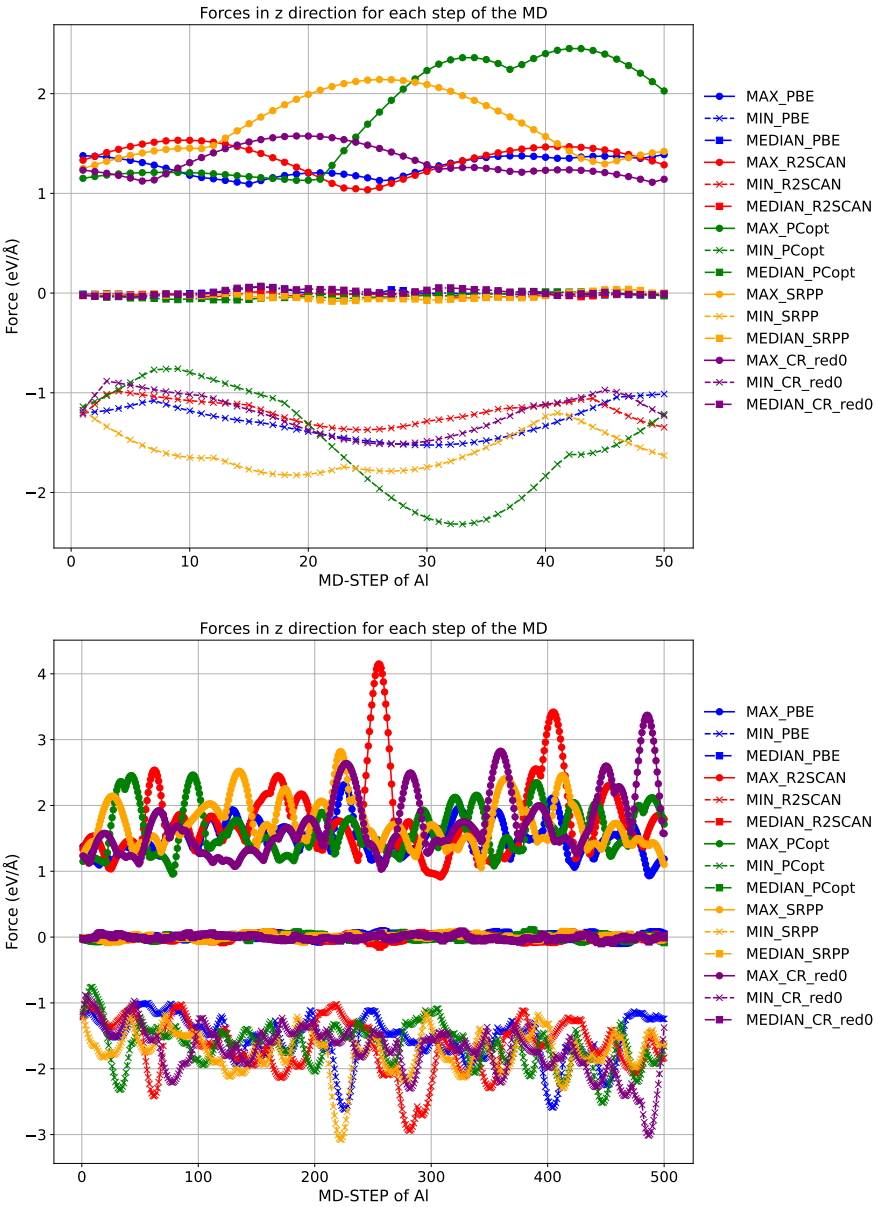


FIG. 4. Maximum, minimum, and median forces in the z direction for the first 50 and 500 steps of the molecular dynamics simulation of aluminum, calculated with different functionals. Top: 50 steps, Bottom: 500 steps.

VI. EXCHANGE-CORRELATION ENERGY ERRORS FOR ATOMS

This section shows exchange-correlation energies for the first 18 neutral atoms as calculated by r^{2}SCAN-L deorbitalized using RPP and SRPP in comparison with benchmark values from Ref. 8 and OEP results obtained with the OPMKS code. [9] As shown in Table XIV, the use of the CR switching function leads to a modest increase in the mean absolute percentage error (from approximately 2.1% to 2.8% for SRPP). These results illustrate the limited impact on the atomic exchange-correlation energy norm of our modification of the switching function from RPP to SRPP.

TABLE XIV. Exchange-correlation energies in Hartree of atoms for $Z \leq 18$, for r^{2}SCAN-L(RPP) and (SRPP) deorbitalized metaGGAs, compared to benchmark quantum chemistry calculations. "Bench" values are the sum of exact exchange from the OPMKS code [9] and correlation energies from Ref. 8. PE is the percentage error with respect to benchmark. The last column is percent difference between the DFT results using RPP and SRPP deorbitalizers.

Atom	Z	RPP(Hartree)	SRPP(Hartree)	Bench	RPP-PE	SRPP-PE	(SRPP vs RPP)-PE
H	1	-0.3056	-0.3013	-0.3125	-2.19	-3.57	-1.41
He	2	-1.0397	-1.0275	-1.0678	-2.63	-3.77	-1.17
Li	3	-1.7845	-1.766	-1.8257	-2.26	-3.27	-1.04
Be	4	-2.691	-2.6625	-2.7598	-2.49	-3.52	-1.06
B	5	-3.8018	-3.7614	-3.8677	-1.70	-2.75	-1.06
C	6	-5.1111	-5.0637	-5.2023	-1.75	-2.66	-0.93
N	7	-6.6323	-6.5837	-6.7604	-1.89	-2.61	-0.73
O	8	-8.2715	-8.2136	-8.4385	-1.98	-2.66	-0.70
F	9	-10.1183	-10.0576	-10.3271	-2.02	-2.61	-0.60
Ne	10	-12.1905	-12.1299	-12.495	-2.44	-2.92	-0.50
Na	11	-14.0688	-14.0157	-14.4091	-2.36	-2.73	-0.38
Mg	12	-16.0548	-15.9922	-16.4264	-2.26	-2.64	-0.39
Al	13	-18.1596	-18.079	-18.5329	-2.01	-2.45	-0.44
Si	14	-20.3753	-20.2881	-20.7781	-1.94	-2.36	-0.43
P	15	-22.7142	-22.6243	-23.1741	-1.98	-2.37	-0.40
S	16	-25.1243	-25.0288	-25.6002	-1.86	-2.23	-0.38
Cl	17	-27.6549	-27.5567	-28.1689	-1.82	-2.17	-0.36
Ar	18	-30.3367	-30.2150	-30.908	-1.85	-2.24	-0.40

VII. CONVERGENCE OF THE EXCHANGE POTENTIAL

To assess the sensitivity of the RPP and SRPP exchange potentials to the quality of the numerical radial grid, we performed a systematic convergence study for the hydrogen atom. The exchange potential was evaluated using increasingly dense logarithmic radial grids, ranging from 100 to 10 000 radial points. The results for RPP and SRPP are shown in Fig. 5.

For coarse grids (fewer than approximately 300 points), both RPP and SRPP exhibit noticeable oscillations in the exchange potential. As the number of grid points is increased, those spurious oscillations diminish rapidly. In the case of RPP, the results obtained with 700, 1000, 5000, and 10,000 points are visually indistinguishable across the entire radial domain, indicating numerical convergence by approximately 700 points. The SRPP exchange potential shows a similar pattern, reaching practical convergence at the same grid density.

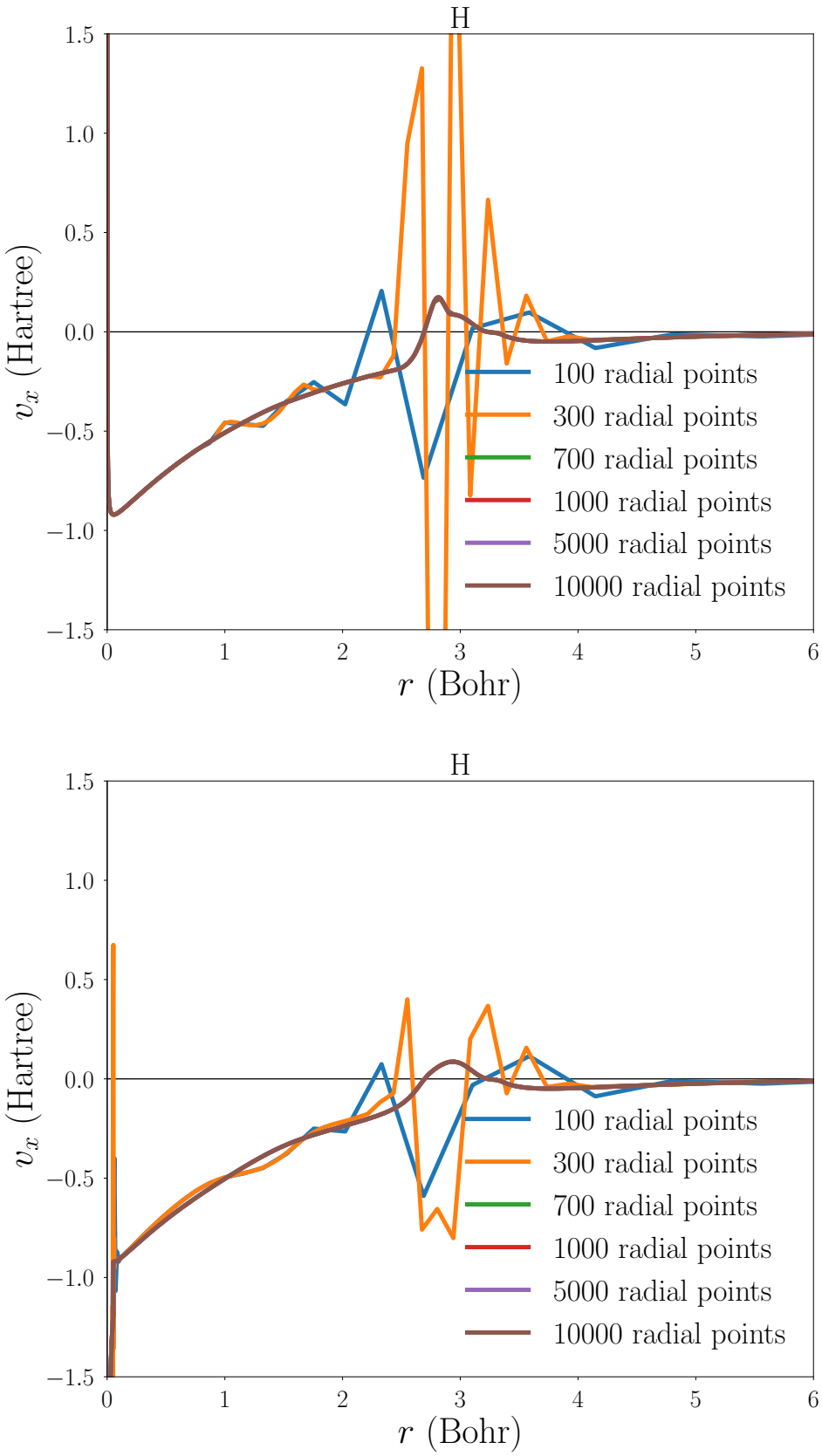


FIG. 5. Convergence of the exchange potential for the hydrogen atom with respect to the number of radial grid points. Top: RPP, Bottom: SRPP.

Acknowledgement: Work supported by U.S. National Science Foundation grant DMR-1912618.

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