Meta-GGA Performance in Solids at Almost GGA Cost
Supplemental Material

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In this supplementary material we present the individual calculated results for each one of the systems in the different test sets. Experimental results are taken from references [S1–S4]. Enthalpies of formation found in the active thermochemical tables [S4] were preferred over those found in reference [S1].

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TABLE S1: r^{2}SCAN standard enthalpies of formation (ΔH_f) in kcal/mol as a function of grid density denoted by NWChem keyword.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
LiH	36.406	36.358	36.365	36.367	36.368	33.300
^{2}BeH	72.394	72.416	72.400	72.402	72.403	81.700
^{2}CH	145.203	145.262	145.246	145.247	145.246	142.500
CH_2 ($^3B_1$)	87.359	87.401	87.382	87.381	87.381	93.600
CH_2 ($^1A_1$)	109.018	109.113	109.087	109.080	109.079	102.600
$^3CH_3$	31.082	31.116	31.096	31.094	31.093	35.000
CH_4	−17.053	−16.954	−16.979	−16.986	−16.987	−17.800
^{3}NH	84.948	84.795	84.818	84.817	84.818	85.800
NH_2 ($^2B_1$)	44.109	43.882	43.948	43.937	43.938	44.500
NH_3	−6.373	−6.667	−6.584	−6.594	−6.594	−10.900
^{2}OH	7.786	7.949	7.897	7.907	7.905	9.000
H_2O	−54.246	−54.040	−54.092	−54.082	−54.083	−57.800
HF	−61.348	−61.579	−61.576	−61.577	−61.578	−65.200
SiH_2 ($^1A_1$)	67.635	67.662	67.657	67.658	67.657	65.200
SiH_2 ($^3B_1$)	78.689	78.687	78.683	78.683	78.683	86.200
$^2SiH_3$	43.321	43.307	43.306	43.306	43.306	47.900
SiH_4	8.064	8.047	8.049	8.049	8.049	8.200
$^2PH_2$	30.282	30.292	30.297	30.297	30.297	33.100
PH_3	2.894	2.907	2.913	2.912	2.912	1.300
H_2S	−4.797	−4.796	−4.805	−4.805	−4.805	−4.900
HCl	−21.705	−21.704	−21.697	−21.698	−21.698	−22.000
Li_2	58.043	57.923	57.939	57.944	57.945	51.600
LiF	−75.375	−75.252	−75.222	−75.224	−75.224	−80.100
HC≡CH	56.988	57.310	57.295	57.290	57.287	54.600
$H_2C{=}CH_2$	12.901	13.278	13.278	13.270	13.267	12.500
$H_3C{-}CH_3$	−20.318	−19.899	−19.889	−19.900	−19.903	−20.100
CN	108.275	108.268	108.294	108.282	108.281	105.200
HCN	36.212	36.374	36.363	36.343	36.342	30.900
CO	−22.563	−22.471	−22.501	−22.493	−22.495	−26.400
^{2}HCO	6.383	6.439	6.373	6.379	6.376	10.000
H_2CO	−25.509	−25.425	−25.490	−25.489	−25.492	−26.100
CH_3OH	−46.367	−46.476	−46.550	−46.548	−46.551	−48.000
N_2	9.200	8.566	8.721	8.705	8.705	0.000
H_2NNH_2	33.144	32.395	32.430	32.406	32.407	23.300
NO	22.250	22.210	22.180	22.181	22.180	21.800
$^3O_2$	−9.713	−9.387	−9.513	−9.490	−9.493	0.000
H_2O_2	−31.828	−31.244	−31.292	−31.278	−31.281	−32.400
F_2	−0.158	−0.516	−0.542	−0.540	−0.543	0.000
CO_2	−99.524	−99.649	−99.740	−99.727	−99.731	−94.000
Na_2	37.340	37.353	37.361	37.360	37.361	34.000
Si_2	140.044	140.053	140.048	140.048	140.048	139.900
P_2	38.928	38.894	38.899	38.899	38.899	34.300
$^3S_2$	21.585	21.558	21.555	21.555	21.554	30.700
Cl_2	−1.175	−1.174	−1.174	−1.175	−1.174	0.000
NaCl	−42.211	−42.208	−42.209	−42.210	−42.212	−43.600
SiO	−19.972	−19.605	−19.635	−19.627	−19.628	−24.600
CS	69.391	69.389	69.390	69.395	69.394	66.900
SO	−5.653	−5.760	−5.792	−5.787	−5.789	1.200
ClO	18.930	18.842	18.804	18.817	18.815	24.300
ClF	−13.496	−13.507	−13.515	−13.513	−13.515	−13.300
Si_2H_6	16.225	16.108	16.108	16.112	16.111	19.100
CH_3Cl	−20.382	−20.547	−20.542	−20.539	−20.540	−19.600
$H_3C{-}SH$	−6.386	−6.340	−6.359	−6.360	−6.362	−5.500
HOCl	−18.530	−18.240	−18.268	−18.260	−18.261	−18.400
SO_2	−72.542	−72.597	−72.675	−72.659	−72.663	−71.000
BF_3	−273.112	−273.726	−273.730	−273.730	−273.733	−271.400
BCl_3	−106.311	−106.303	−106.291	−106.301	−106.302	−96.300
AlF_3	−286.903	−286.256	−286.276	−286.280	−286.284	−289.000
$AlCl_3$	−147.854	−147.942	−147.938	−147.939	−147.945	−139.700
CF_4	−228.729	−229.497	−229.510	−229.512	−229.518	−223.100
CCl_4	−29.147	−29.317	−29.326	−29.328	−29.332	−22.900

TABLE S1: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
OCS	−42.304	−42.102	−42.156	−42.143	−42.145	−33.100
CS_2	16.973	16.922	16.912	16.916	16.914	28.000
F_2CO	−151.254	−151.363	−151.357	−151.350	−151.356	−145.000
SiF_4	−382.093	−381.420	−381.343	−381.348	−381.353	−386.000
$SiCl_4$	−165.400	−165.613	−165.546	−165.546	−165.551	−158.400
NNO	15.628	14.809	14.873	14.877	14.876	19.700
ClNO	5.945	5.303	5.357	5.363	5.362	12.600
NF_3	−40.314	−40.566	−40.574	−40.578	−40.582	−31.600
PF_3	−225.572	−226.231	−226.171	−226.170	−226.175	−229.100
O_3	28.336	29.314	29.223	29.252	29.247	33.900
F_2O	−0.771	−0.940	−1.025	−1.012	−1.016	5.900
ClF_3	−51.399	−52.165	−52.035	−52.042	−52.046	−38.000
$F_2C{=}CF_2$	−169.751	−170.690	−170.519	−170.532	−170.539	−161.300
$Cl_2C{=}CCl_2$	−14.961	−14.882	−14.833	−14.835	−14.841	−5.500
$F_3C{-}CN$	−121.433	−121.512	−121.750	−121.758	−121.763	−118.400
$HC{\equiv}C{-}CH_3$	44.636	44.634	44.573	44.558	44.553	44.400
$H_2C{=}C{=}CH_2$	41.526	41.679	41.751	41.755	41.755	45.400
C_3H_4 (cyclopropene)	65.506	65.529	65.521	65.515	65.511	67.800
$H_2C{=}CH{-}CH_3$	3.456	4.262	4.171	4.182	4.177	4.800
C_3H_6 (cyclopropane)	9.708	10.335	10.333	10.331	10.326	12.800
$CH_3{-}CH_2{-}CH_3$	−26.056	−25.155	−25.271	−25.257	−25.263	−25.100
C_4H_6 (Z-1,3-butadiene)	24.534	24.163	24.231	24.251	24.243	26.400
C_4H_6 (2-butyne)	33.929	33.525	33.584	33.598	33.591	34.800
C_4H_6 (methylenecyclopropane)	40.208	41.303	41.175	41.189	41.183	47.900
C_4H_6 (bicyclo[1.1.0]butane)	47.951	48.187	48.312	48.323	48.323	51.900
C_4H_6 (cyclobutene)	36.479	36.668	36.819	36.788	36.788	38.200
C_4H_8 (cyclobutane)	4.880	5.450	5.232	5.201	5.201	6.600
C_4H_8 (isobutene)	−6.283	−5.174	−5.310	−5.295	−5.302	−4.100
C_4H_{10} (trans butane)	−30.341	−30.614	−30.529	−30.574	−30.582	−30.100
C_4H_{10} (isobutane)	−33.264	−32.052	−32.206	−32.189	−32.197	−32.200
C_5H_8 (spiropentane)	36.242	37.695	37.503	37.524	37.515	44.300
C_6H_6 (benzene)	10.629	10.770	10.428	10.400	10.395	19.900
CH_2F_2	−109.420	−109.052	−109.017	−109.027	−109.031	−107.700
CHF_3	−170.840	−170.310	−170.247	−170.259	−170.265	−166.300
CH_2Cl_2	−25.443	−25.535	−25.531	−25.529	−25.532	−22.600
$CHCl_3$	−29.174	−29.255	−29.251	−29.249	−29.253	−24.500
CH_3NH_2	5.436	5.713	5.696	5.679	5.678	−5.200
CH_3CN	20.111	20.155	20.218	20.212	20.210	18.000
CH_3NO_2 (nitromethane)	−26.257	−25.799	−25.879	−25.880	−25.883	−17.900
CH_3ONO (methyl nitrite)	−20.787	−21.374	−21.310	−21.288	−21.294	−16.100
CH_3SiH_3	−6.786	−6.951	−7.012	−7.009	−7.010	−7.000
HCO_2H	−92.531	−92.947	−93.060	−93.043	−93.047	−90.400
HCO_2CH_3	−89.239	−89.516	−89.562	−89.538	−89.540	−85.500
CH_3CONH_2	−58.972	−58.962	−58.889	−58.879	−58.881	−57.000
C_2H_5N (aziridine)	29.847	30.292	30.306	30.291	30.289	30.200
NCCN (cyanogen)	77.821	77.446	77.589	77.588	77.585	74.100
$NH(CH_3)_2$	−2.276	−1.797	−1.717	−1.725	−1.725	−4.300
$CH_3CH_2NH_2$	−9.116	−9.495	−9.436	−9.445	−9.446	−11.300
$H_2C{=}C{=}O$ (ketene)	−18.258	−17.632	−17.674	−17.673	−17.677	−11.600
C_2H_4O (oxirane)	−15.470	−15.069	−15.121	−15.115	−15.119	−12.600
CH_3CHO	−41.837	−41.173	−41.216	−41.208	−41.213	−39.500
$O{=}CH{-}CH{=}O$	−53.762	−52.821	−52.952	−52.933	−52.938	−50.800
CH_3CH_2OH	−55.533	−55.581	−55.493	−55.501	−55.502	−56.100
$(CH_3)_2O$	−44.242	−44.160	−44.144	−44.133	−44.135	−44.000
C_2H_4S (thiooxirane)	14.763	15.148	15.131	15.128	15.124	19.600
$(CH_3)_2S{=}O$	−40.910	−40.538	−40.599	−40.595	−40.600	−36.200
CH_3CH_2SH	−11.995	−12.068	−12.115	−12.122	−12.126	−11.100
$(CH_3)_2S$	−10.819	−10.872	−10.924	−10.930	−10.933	−8.900
$H_2C{=}CHF$	−36.340	−35.798	−35.869	−35.880	−35.884	−34.000
CH_3CH_2Cl	−28.423	−28.386	−28.389	−28.394	−28.398	−26.600
$H_2C{=}CHCl$	2.748	2.762	2.763	2.758	2.754	5.200
$H_2C{=}CHCN$	45.736	45.853	46.029	46.037	46.033	43.200

TABLE S1: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
$(CH_3)_2C{=}O$	−55.598	−54.507	−54.655	−54.629	−54.636	−51.700
CH_3CO_2H	−106.801	−106.938	−106.945	−106.946	−106.949	−103.400
CH_3CFO	−110.706	−109.882	−109.992	−109.995	−110.001	−105.700
CH_3COCl	−64.882	−64.592	−64.639	−64.632	−64.638	−57.700
$CH_3CH_2CH_2Cl$	−33.528	−33.497	−33.673	−33.689	−33.691	−31.500
$(CH_3)_2CHOH$	−65.817	−65.102	−65.197	−65.178	−65.185	−65.200
$CH_3{-}O{-}CH_2CH_3$	−52.629	−53.057	−52.989	−52.970	−52.977	−51.700
$(CH_3)_3N$	−4.473	−4.256	−4.146	−4.153	−4.153	−6.600
C_4H_4O (furan)	−15.574	−15.506	−15.452	−15.439	−15.441	−8.300
C_4H_4S (thiophene)	17.945	19.014	18.908	18.919	18.911	27.500
C_4H_5N (pyrrole)	20.476	20.370	20.528	20.530	20.531	25.900
C_5H_5N (pyridine)	25.984	26.011	25.910	25.887	25.882	33.600
H_2	2.028	2.029	2.029	2.029	2.029	0.000
^2SH	32.437	32.441	32.444	32.443	32.443	34.200
$^2C{\equiv}CH$	134.237	134.482	134.499	134.490	134.489	135.800
$HC{=}CH_2$ ($^2A'$)	65.868	66.153	66.145	66.138	66.136	71.000
$CH_3C{=}O$ ($^2A'$)	−8.546	−7.957	−8.020	−8.015	−8.019	−2.400
$CH_2{-}OH$ (^2A)	−7.773	−7.838	−7.901	−7.898	−7.900	−4.000
CH_3O ($^2A'$)	−1.033	−0.919	−1.002	−1.001	−1.004	5.200
CH_3CH_2O ($^2A''$)	−11.150	−10.791	−10.757	−10.757	−10.763	−2.900
CH_3S ($^2A'$)	25.605	25.466	25.428	25.432	25.430	29.800
CH_2CH_3 ($^2A'$)	23.142	23.500	23.481	23.478	23.476	28.600
$(CH_3)_2CH$ ($^2A'$)	13.896	14.685	14.605	14.610	14.606	21.100
$^2C(CH_3)_3$	4.248	5.346	5.227	5.236	5.230	12.000
NO_2 ($^2A_1$)	−3.604	−3.190	−3.228	−3.219	−3.221	8.100
$CH_3CH{=}C{=}CH_2$	35.408	34.516	34.584	34.597	34.596	38.800
C_5H_8 (isoprene)	15.867	15.437	15.510	15.534	15.524	18.000
C_5H_{10} (cyclopentane twist)	−21.423	−20.283	−20.114	−20.089	−20.099	−18.500
C_5H_{12} (n-pentane)	−35.187	−35.971	−35.765	−35.814	−35.825	−35.000
$C(CH_3)_4$ (neopentane)	−41.266	−39.641	−39.815	−39.786	−39.796	−40.100
C_6H_8 (1,3-cyclohexadiene)	21.846	21.957	21.606	21.571	21.568	25.400
C_6H_8 (1,4-cyclohexadiene)	22.082	22.147	21.808	21.775	21.772	25.000
C_6H_{12} (cyclohexane chair)	−30.503	−30.526	−30.889	−30.897	−30.900	−29.400
C_6H_{14} (n-hexane)	−42.137	−40.763	−41.063	−41.094	−41.087	−39.900
C_6H_{14} (3-methylpentane)	−40.275	−41.192	−40.945	−41.008	−41.021	−41.100
$C_6H_5{-}CH_3$ (toluene)	0.628	2.578	2.182	2.187	2.172	12.000
C_7H_{16} (n-heptane)	−47.699	−46.748	−46.408	−46.322	−46.340	−44.800
C_8H_8 (cyclooctatetraene)	66.690	64.932	65.048	65.070	65.069	70.700
C_8H_{18} (n-octane)	−53.156	−52.068	−51.681	−51.583	−51.604	−49.800
$C_{10}H_8$ (naphtalene)	18.574	16.936	17.335	17.418	17.397	35.900
$C_{10}H_8$ (azulene)	51.962	49.697	50.097	50.159	50.160	69.100
$CH_3CO_2CH_3$ (Z-methylacetate)	−102.242	−102.879	−102.925	−102.891	−102.899	−98.400
$(CH_3)_3COH$ (t-butanol)	−75.542	−74.519	−74.652	−74.627	−74.637	−74.700
$C_6H_5NH_2$ (aniline)	11.638	11.011	11.220	11.144	11.133	20.800
C_6H_5OH (phenol)	−32.857	−33.556	−33.534	−33.499	−33.512	−22.300
C_4H_6O (divinyl ether)	−7.463	−7.517	−7.407	−7.407	−7.407	−3.300
C_4H_8O (tetrahydrofuran)	−45.913	−45.851	−45.758	−45.742	−45.744	−44.000
C_5H_8O (cyclopentanone)	−52.926	−51.576	−51.414	−51.379	−51.379	−45.900
$C_6H_4O_2$ (benzoquinone)	−39.124	−38.503	−38.779	−38.775	−38.783	−29.400
$C_6H_4N_2$ (pyrimidine)	39.204	39.344	39.259	39.242	39.238	46.800
$(CH_3)_2SO_2$	−95.054	−95.529	−95.584	−95.575	−95.579	−89.200
C_6H_5Cl (chlorobenzene)	1.408	0.151	0.272	0.249	0.249	12.500
$NC(CH_2)_2CN$ (succinonitrile)	55.244	54.529	54.656	54.661	54.662	50.100
$C_4H_4N_2$ (pyrazine)	44.033	43.352	43.414	43.397	43.390	46.900
C_4H_4O (3-butyn-2-one)	15.354	15.136	15.209	15.243	15.234	15.600
C_4H_6O (E-crotonaldehyde)	−28.763	−29.378	−29.476	−29.433	−29.444	−24.000
$C_4H_6O_3$ (acetic anhydride)	−147.157	−146.984	−146.696	−146.705	−146.708	−136.800
C_4H_6S (2,5-dihydrothiophene)	14.919	15.818	15.926	15.941	15.933	20.800
$(CH_3)_2CHCN$	8.582	9.257	9.208	9.223	9.217	5.600
C_4H_8O (methyl ethyl ketone)	−60.080	−60.337	−60.291	−60.326	−60.335	−57.100
$(CH_3)_2CHCHO$	−53.650	−52.259	−52.391	−52.368	−52.377	−51.600
$C_4H_8O_2$ (1,4-dioxane)	−78.303	−78.613	−78.662	−78.668	−78.674	−75.500

TABLE S1: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
C_4H_8S (tetrahydrothiophene)	−12.060	−10.856	−10.989	−10.973	−10.981	−8.200
$(CH_3)_3CCl$	−46.727	−45.566	−45.703	−45.687	−45.696	−43.500
C_4H_9Cl (n-butyl chloride)	−39.667	−38.608	−38.820	−38.873	−38.872	−37.000
C_4H_9N (tetrahydropyrrole)	−0.958	−0.365	−0.179	−0.170	−0.170	−0.800
$C_4H_9NO_2$ (2-nitrobutane)	−47.872	−47.568	−47.455	−47.463	−47.472	−39.100
$(CH_3CH_2)_2O$	−61.693	−61.781	−61.702	−61.705	−61.705	−60.300
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	−94.781	−95.092	−95.125	−95.090	−95.099	−93.100
$(CH_3)_3CSH$	−27.194	−27.352	−27.459	−27.477	−27.485	−26.200
$C_4H_{10}S_2$ (diethyl disulfide)	−22.432	−22.240	−22.451	−22.454	−22.464	−17.900
$(CH_3)_3CNH_2$	−27.568	−26.304	−26.391	−26.384	−26.392	−28.900
$(CH_3)_4Si$	−53.909	−53.971	−54.179	−54.180	−54.181	−55.700
C_5H_6S (2-methyl thiophene)	9.868	11.094	10.808	10.740	10.742	20.000
C_5H_7N (N-methyl pyrrole)	19.564	18.795	18.928	18.949	18.939	24.600
$C_5H_{10}O$ (tetrahydropyran)	−55.300	−55.221	−55.538	−55.558	−55.561	−53.400
$(CH_3CH_2)_2C{=}O$	−65.337	−66.061	−65.880	−65.922	−65.934	−61.600
$C_5H_{10}O_2$ (isopropyl acetate)	−121.286	−120.747	−120.557	−120.534	−120.534	−115.100
$C_5H_{10}S$ (tetrahydrothiopyran)	−17.283	−18.098	−18.388	−18.404	−18.406	−15.200
$C_5H_{11}N$ (piperidine)	−10.241	−10.157	−10.402	−10.432	−10.434	−11.300
$C_5H_{12}O$ (t-butyl methyl ether)	−68.117	−68.618	−68.557	−68.526	−68.537	−67.800
$C_6H_4F_2$ (1,3-difluorobenzene)	−89.149	−88.526	−88.644	−88.650	−88.657	−73.900
$C_6H_4F_2$ (1,4-difluorobenzene)	−86.649	−87.224	−87.734	−87.758	−87.765	−73.300
C_6H_5F (fluorobenzene)	−39.565	−39.185	−39.416	−39.433	−39.439	−27.400
$C_6H_{14}O$ (diisopropyl ether)	−77.872	−77.945	−77.828	−77.841	−77.838	−76.300
PF_5	−380.506	−380.274	−380.272	−380.252	−380.259	−381.100
SF_6	−303.951	−303.674	−303.635	−303.617	−303.624	−291.700
P_4	9.867	9.912	9.930	9.930	9.931	14.100
SO_3	−102.376	−102.465	−102.579	−102.555	−102.560	−94.600
SCl_2	−9.255	−9.268	−9.248	−9.247	−9.250	−4.200
$POCl_3$	−141.200	−140.869	−140.875	−140.867	−140.871	−133.800
PCl_5	−99.213	−99.244	−99.204	−99.207	−99.211	−86.100
Cl_2O_2S	−97.558	−96.931	−97.016	−97.000	−97.006	−84.800
PCl_3	−74.848	−74.831	−74.783	−74.784	−74.787	−69.000
Cl_2S_2	−18.055	−18.132	−18.126	−18.126	−18.129	−4.000
$SiCl_2$ ($^1A_1$)	−42.784	−42.773	−42.737	−42.738	−42.740	−40.300
CF_3Cl	−177.683	−177.620	−177.697	−177.682	−177.686	−169.700
C_2F_6	−331.119	−332.885	−332.625	−332.631	−332.641	−320.900
$^2CF_3$	−121.565	−122.089	−122.127	−122.123	−122.128	−111.800
$^2C_6H_5$ (phenyl radical)	65.567	65.664	65.361	65.331	65.325	80.500
M.D.	−3.220	−3.134	−3.149	−3.147	−3.151	
M.A.D.	4.530	4.476	4.491	4.489	4.491	

TABLE S2: r^{2}SCAN-L standard enthalpies of formation (ΔH_f) in kcal/mol as in preceding Table.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
LiH	36.977	37.132	37.099	37.109	37.113	33.300
^{2}BeH	71.667	71.826	71.727	71.715	71.717	81.700
^{2}CH	142.967	142.939	142.899	142.897	142.897	142.500
CH_2 ($^3B_1$)	89.005	89.059	89.023	89.023	89.022	93.600
CH_2 ($^1A_1$)	107.412	107.495	107.417	107.422	107.420	102.600
$^3CH_3$	33.259	33.297	33.251	33.252	33.251	35.000
CH_4	−13.412	−13.377	−13.453	−13.443	−13.447	−17.800
^{3}NH	80.919	80.942	80.930	80.954	80.955	85.800
NH_2 ($^2B_1$)	39.991	39.849	39.895	39.917	39.917	44.500
NH_3	−9.326	−9.385	−9.341	−9.316	−9.314	−10.900
^{2}OH	6.621	6.832	6.791	6.773	6.775	9.000
H_2O	−54.098	−53.717	−53.754	−53.776	−53.774	−57.800
HF	−59.472	−59.852	−59.863	−59.851	−59.846	−65.200
SiH_2 ($^1A_1$)	68.483	68.515	68.505	68.505	68.503	65.200
SiH_2 ($^3B_1$)	80.132	80.117	80.108	80.106	80.105	86.200
$^2SiH_3$	45.967	45.942	45.942	45.945	45.943	47.900
SiH_4	12.494	12.487	12.498	12.501	12.500	8.200
$^2PH_2$	30.771	30.757	30.767	30.770	30.769	33.100
PH_3	4.562	4.554	4.560	4.561	4.559	1.300
H_2S	−2.936	−2.932	−2.942	−2.944	−2.945	−4.900
HCl	−20.277	−20.304	−20.274	−20.269	−20.273	−22.000
Li_2	57.100	57.335	57.283	57.313	57.323	51.600
LiF	−72.449	−72.334	−72.343	−72.314	−72.305	−80.100
HC≡CH	58.444	58.835	58.896	58.891	58.885	54.600
$H_2C{=}CH_2$	16.139	16.592	16.629	16.660	16.652	12.500
$H_3C{-}CH_3$	−14.858	−14.336	−14.313	−14.285	−14.294	−20.100
CN	101.434	101.636	101.593	101.621	101.622	105.200
HCN	31.991	32.552	32.376	32.403	32.406	30.900
CO	−22.408	−22.388	−22.429	−22.434	−22.437	−26.400
^{2}HCO	5.752	5.902	5.801	5.783	5.784	10.000
H_2CO	−24.893	−24.742	−24.870	−24.878	−24.878	−26.100
CH_3OH	−43.608	−43.919	−44.064	−44.065	−44.066	−48.000
N_2	−0.112	−0.343	−0.293	−0.240	−0.236	0.000
H_2NNH_2	25.342	24.557	24.409	24.446	24.452	23.300
NO	14.644	15.152	15.016	15.020	15.025	21.800
$^3O_2$	−13.558	−12.839	−12.932	−12.961	−12.954	0.000
H_2O_2	−36.075	−35.332	−35.319	−35.349	−35.348	−32.400
F_2	−4.188	−4.597	−4.681	−4.665	−4.657	0.000
CO_2	−96.927	−97.335	−97.406	−97.443	−97.443	−94.000
Na_2	37.438	37.539	37.546	37.546	37.547	34.000
Si_2	135.944	135.924	135.910	135.912	135.909	139.900
P_2	37.059	36.917	36.922	36.922	36.924	34.300
$^3S_2$	22.303	22.336	22.321	22.318	22.318	30.700
Cl_2	−1.747	−1.659	−1.638	−1.638	−1.642	0.000
NaCl	−38.970	−39.101	−39.092	−39.092	−39.094	−43.600
SiO	−19.740	−19.077	−19.127	−19.147	−19.147	−24.600
CS	68.291	68.151	68.213	68.214	68.212	66.900
SO	−5.711	−6.094	−6.155	−6.155	−6.152	1.200
ClO	16.322	16.013	15.988	15.975	15.978	24.300
ClF	−14.714	−14.528	−14.541	−14.552	−14.546	−13.300
Si_2H_6	23.714	23.575	23.576	23.590	23.588	19.100
CH_3Cl	−16.905	−17.443	−17.368	−17.375	−17.378	−19.600
$H_3C{-}SH$	−2.514	−2.638	−2.605	−2.615	−2.616	−5.500
HOCl	−20.634	−20.228	−20.223	−20.217	−20.218	−18.400
SO_2	−71.195	−71.324	−71.334	−71.374	−71.370	−71.000
BF_3	−260.625	−261.252	−261.174	−261.172	−261.162	−271.400
BCl_3	−100.523	−100.479	−100.462	−100.432	−100.449	−96.300
AlF_3	−273.958	−273.830	−273.888	−273.840	−273.823	−289.000
$AlCl_3$	−139.107	−139.078	−138.937	−138.944	−138.947	−139.700
CF_4	−215.380	−216.598	−216.601	−216.622	−216.605	−223.100
CCl_4	−26.464	−27.076	−27.082	−27.076	−27.090	−22.900
OCS	−40.060	−40.224	−40.228	−40.242	−40.242	−33.100

TABLE S2: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
CS_2	18.840	18.691	18.744	18.741	18.734	28.000
F_2CO	−144.175	−144.597	−144.431	−144.422	−144.412	−145.000
SiF_4	−362.353	−362.471	−362.303	−362.247	−362.228	−386.000
$SiCl_4$	−154.607	−154.490	−154.400	−154.410	−154.409	−158.400
NNO	6.177	5.008	5.069	5.090	5.097	19.700
ClNO	−2.294	−3.255	−3.174	−3.157	−3.149	12.600
NF_3	−46.146	−45.689	−45.797	−45.791	−45.778	−31.600
PF_3	−215.477	−216.323	−216.130	−216.138	−216.129	−229.100
O_3	17.241	18.703	18.632	18.637	18.638	33.900
F_2O	−7.630	−7.828	−7.969	−7.973	−7.964	5.900
ClF_3	−52.390	−52.963	−52.703	−52.657	−52.647	−38.000
$F_2C{=}CF_2$	−159.787	−160.722	−160.268	−160.215	−160.212	−161.300
$Cl_2C{=}CCl_2$	−11.325	−10.903	−10.933	−10.985	−10.982	−5.500
$F_3C{-}CN$	−116.304	−116.729	−117.277	−117.285	−117.269	−118.400
$HC{\equiv}C{-}CH_3$	49.597	49.384	49.283	49.243	49.231	44.400
$H_2C{=}C{=}CH_2$	46.199	45.868	46.105	46.142	46.138	45.400
C_3H_4 (cyclopropene)	70.109	69.979	69.985	69.955	69.951	67.800
$H_2C{=}CH{-}CH_3$	8.924	10.348	10.169	10.214	10.202	4.800
C_3H_6 (cyclopropane)	16.800	17.578	17.674	17.649	17.636	12.800
$CH_3{-}CH_2{-}CH_3$	−18.774	−17.242	−17.429	−17.377	−17.389	−25.100
C_4H_6 (Z-1,3-butadiene)	32.142	30.376	30.642	30.579	30.584	26.400
C_4H_6 (2-butyne)	42.775	40.974	41.258	41.189	41.193	34.800
C_4H_6 (methylenecyclopropane)	47.405	49.325	49.082	49.143	49.129	47.900
C_4H_6 (bicyclo[1.1.0]butane)	57.184	56.752	57.096	57.164	57.155	51.900
C_4H_6 (cyclobutene)	43.687	43.213	43.644	43.602	43.594	38.200
C_4H_8 (cyclobutane)	13.658	14.046	13.627	13.577	13.568	6.600
C_4H_8 (isobutene)	1.552	3.513	3.261	3.324	3.308	−4.100
C_4H_{10} (trans butane)	−18.951	−20.668	−20.457	−20.450	−20.441	−30.100
C_4H_{10} (isobutane)	−23.857	−21.811	−22.061	−21.991	−22.006	−32.200
C_5H_8 (spiropentane)	46.977	49.452	49.135	49.220	49.204	44.300
C_6H_6 (benzene)	21.908	21.971	21.217	21.099	21.118	19.900
CH_2F_2	−102.637	−102.722	−102.658	−102.634	−102.627	−107.700
CHF_3	−160.719	−160.853	−160.723	−160.690	−160.677	−166.300
CH_2Cl_2	−22.063	−22.489	−22.449	−22.454	−22.461	−22.600
$CHCl_3$	−26.011	−26.414	−26.390	−26.388	−26.399	−24.500
CH_3NH_2	4.061	4.880	4.698	4.732	4.731	−5.200
CH_3CN	19.457	19.539	19.699	19.695	19.687	18.000
CH_3NO_2 (nitromethane)	−30.411	−29.646	−29.862	−29.859	−29.858	−17.900
CH_3ONO (methyl nitrite)	−26.273	−27.226	−27.070	−27.055	−27.044	−16.100
CH_3SiH_3	0.901	0.310	0.180	0.193	0.194	−7.000
HCO_2H	−89.262	−90.307	−90.467	−90.474	−90.474	−90.400
HCO_2CH_3	−84.073	−84.879	−84.832	−84.802	−84.806	−85.500
CH_3CONH_2	−57.207	−56.856	−56.649	−56.620	−56.620	−57.000
C_2H_5N (aziridine)	30.251	31.200	31.187	31.193	31.189	30.200
NCCN (cyanogen)	68.916	68.485	68.744	68.761	68.769	74.100
$NH(CH_3)_2$	−1.393	−0.270	−0.183	−0.131	−0.133	−4.300
$CH_3CH_2NH_2$	−6.804	−7.788	−7.754	−7.713	−7.704	−11.300
$H_2C{=}C{=}O$ (ketene)	−15.236	−14.565	−14.543	−14.522	−14.529	−11.600
C_2H_4O (oxirane)	−11.595	−11.045	−11.007	−11.038	−11.043	−12.600
CH_3CHO	−38.120	−37.321	−37.249	−37.276	−37.285	−39.500
$O{=}CH{-}CH{=}O$	−53.116	−51.853	−51.937	−51.979	−51.982	−50.800
CH_3CH_2OH	−50.311	−50.714	−50.408	−50.439	−50.440	−56.100
$(CH_3)_2O$	−39.160	−39.328	−39.205	−39.193	−39.196	−44.000
C_2H_4S (thiooxirane)	19.708	20.082	20.154	20.141	20.133	19.600
$(CH_3)_2S{=}O$	−33.905	−33.325	−33.332	−33.371	−33.375	−36.200
CH_3CH_2SH	−5.812	−5.990	−6.035	−6.069	−6.078	−11.100
$(CH_3)_2S$	−4.668	−4.905	−4.960	−4.990	−4.998	−8.900
$H_2C{=}CHF$	−31.169	−30.702	−30.829	−30.799	−30.799	−34.000
CH_3CH_2Cl	−22.589	−22.776	−22.748	−22.772	−22.779	−26.600
$H_2C{=}CHCl$	6.653	6.451	6.457	6.442	6.436	5.200
$H_2C{=}CHCN$	44.399	44.863	45.239	45.317	45.313	43.200
$(CH_3)_2C{=}O$	−49.296	−47.533	−47.738	−47.702	−47.714	−51.700

TABLE S2: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
CH_3CO_2H	−101.020	−101.444	−101.240	−101.279	−101.282	−103.400
CH_3CFO	−103.513	−102.813	−102.945	−102.928	−102.928	−105.700
CH_3COCl	−59.917	−59.875	−59.871	−59.902	−59.908	−57.700
$CH_3CH_2CH_2Cl$	−25.343	−25.363	−25.765	−25.820	−25.809	−31.500
$(CH_3)_2CHOH$	−58.810	−57.480	−57.592	−57.558	−57.565	−65.200
$CH_3-O-CH_2CH_3$	−44.196	−45.855	−45.418	−45.480	−45.471	−51.700
$(CH_3)_3N$	−0.530	−0.414	−0.238	−0.172	−0.176	−6.600
C_4H_4O (furan)	−8.123	−8.682	−8.373	−8.333	−8.339	−8.300
C_4H_4S (thiophene)	25.355	27.237	27.007	27.076	27.057	27.500
C_4H_5N (pyrrole)	25.306	24.647	24.985	25.051	25.050	25.900
C_5H_5N (pyridine)	30.793	31.067	30.745	30.669	30.685	33.600
H_2	3.364	3.366	3.370	3.370	3.369	0.000
^2SH	33.094	33.088	33.087	33.084	33.084	34.200
$^2C{\equiv}CH$	134.240	134.617	134.666	134.663	134.659	135.800
$HC{=}CH_2$ ($^2A'$)	68.085	68.485	68.542	68.536	68.530	71.000
$CH_3C{=}O$ ($^2A'$)	−6.190	−5.455	−5.431	−5.417	−5.422	−2.400
CH_2-OH (^2A)	−6.152	−6.388	−6.503	−6.514	−6.514	−4.000
CH_3O ($^2A'$)	0.645	0.942	0.770	0.763	0.762	5.200
CH_3CH_2O ($^2A''$)	−7.293	−6.617	−6.388	−6.429	−6.434	−2.900
CH_3S ($^2A'$)	28.833	28.316	28.254	28.251	28.248	29.800
CH_2CH_3 ($^2A'$)	27.591	28.123	28.176	28.166	28.160	28.600
$(CH_3)_2CH$ ($^2A'$)	20.884	22.084	21.907	21.948	21.939	21.100
$^2C(CH_3)_3$	13.687	15.407	15.169	15.228	15.215	12.000
NO_2 ($^2A_1$)	−12.051	−10.986	−11.112	−11.084	−11.077	8.100
$CH_3CH{=}C{=}CH_2$	44.003	40.948	41.426	41.378	41.361	38.800
C_5H_8 (isoprene)	26.262	24.068	24.411	24.328	24.335	18.000
C_5H_{10} (cyclopentane twist)	−11.101	−9.325	−8.879	−8.786	−8.804	−18.500
C_5H_{12} (n-pentane)	−21.279	−23.875	−23.437	−23.447	−23.428	−35.000
$C(CH_3)_4$ (neopentane)	−29.812	−27.125	−27.426	−27.333	−27.353	−40.100
C_6H_8 (1,3-cyclohexadiene)	32.904	33.006	32.214	32.084	32.103	25.400
C_6H_8 (1,4-cyclohexadiene)	33.429	33.490	32.711	32.583	32.601	25.000
C_6H_{12} (cyclohexane chair)	−16.174	−16.094	−17.180	−17.061	−17.043	−29.400
C_6H_{14} (n-hexane)	−28.238	−26.140	−26.569	−26.407	−26.432	−39.900
C_6H_{14} (3-methylpentane)	−23.997	−27.075	−26.551	−26.567	−26.544	−41.100
$C_6H_5-CH_3$ (toluene)	13.161	16.155	15.571	15.414	15.426	12.000
C_7H_{16} (n-heptane)	−31.762	−30.362	−29.600	−29.457	−29.428	−44.800
C_8H_8 (cyclooctatetraene)	81.656	75.629	76.551	76.461	76.428	70.700
C_8H_{18} (n-octane)	−35.091	−33.500	−32.631	−32.467	−32.433	−49.800
$C_{10}H_8$ (naphtalene)	39.091	33.849	34.627	34.810	34.850	35.900
$C_{10}H_8$ (azulene)	72.081	65.179	65.962	66.249	66.186	69.100
$CH_3CO_2CH_3$ (Z-methylacetate)	−93.244	−95.274	−95.065	−95.106	−95.100	−98.400
$(CH_3)_3COH$ (t-butanol)	−66.308	−64.454	−64.629	−64.577	−64.588	−74.700
$C_6H_5NH_2$ (aniline)	21.025	18.529	18.834	18.844	18.853	20.800
C_6H_5OH (phenol)	−19.971	−22.777	−22.462	−22.547	−22.539	−22.300
C_4H_6O (divinyl ether)	−0.559	−1.348	−0.677	−0.763	−0.776	−3.300
C_4H_8O (tetrahydrofuran)	−36.500	−37.083	−36.733	−36.685	−36.690	−44.000
C_5H_8O (cyclopentanone)	−43.551	−41.308	−40.774	−40.705	−40.714	−45.900
$C_6H_4O_2$ (benzoquinone)	−31.870	−30.859	−31.280	−31.419	−31.393	−29.400
$C_6H_4N_2$ (pyrimidine)	37.880	38.888	38.461	38.452	38.440	46.800
$(CH_3)_2SO_2$	−82.728	−83.604	−83.574	−83.638	−83.623	−89.200
C_6H_5Cl (chlorobenzene)	15.115	10.630	11.119	11.243	11.219	12.500
$NC(CH_2)_2CN$ (succinonitrile)	53.429	51.572	51.925	51.984	51.965	50.100
$C_4H_4N_2$ (pyrazine)	42.979	42.012	42.046	42.009	42.000	46.900
C_4H_4O (3-butyn-2-one)	21.602	19.929	20.281	20.204	20.211	15.600
C_4H_6O (E-crotonaldehyde)	−19.945	−22.763	−22.575	−22.648	−22.636	−24.000
$C_4H_6O_3$ (acetic anhydride)	−138.348	−137.715	−136.524	−136.684	−136.693	−136.800
C_4H_6S (2,5-dihydrothiophene)	22.169	23.531	23.857	23.921	23.905	20.800
$(CH_3)_2CHCN$	11.569	13.081	12.949	13.049	13.041	5.600
C_4H_8O (methyl ethyl ketone)	−49.321	−51.257	−51.109	−51.133	−51.124	−57.100
$(CH_3)_2CHCHO$	−45.972	−43.816	−44.021	−43.944	−43.958	−51.600
$C_4H_8O_2$ (1,4-dioxane)	−69.220	−69.750	−69.723	−69.829	−69.807	−75.500
C_4H_8S (tetrahydrothiophene)	−3.199	−1.205	−1.441	−1.370	−1.387	−8.200

TABLE S2: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
$(CH_3)_3CCl$	−37.016	−35.129	−35.361	−35.298	−35.318	−43.500
C_4H_9Cl (n-butyl chloride)	−29.887	−28.068	−28.750	−28.724	−28.744	−37.000
C_4H_9N (tetrahydropyrrole)	3.606	4.677	5.105	5.178	5.173	−0.800
$C_4H_9NO_2$ (2-nitrobutane)	−44.692	−44.788	−44.384	−44.381	−44.366	−39.100
$(CH_3CH_2)_2O$	−51.361	−52.237	−51.552	−51.627	−51.642	−60.300
$CH_3CH(OCH_3)_2$ (dimethyl acetal)	−82.824	−85.263	−84.936	−85.047	−85.039	−93.100
$(CH_3)_3CSH$	−16.223	−16.631	−16.735	−16.802	−16.819	−26.200
$C_4H_{10}S_2$ (diethyl disulfide)	−11.096	−11.068	−11.316	−11.195	−11.214	−17.900
$(CH_3)_3CNH_2$	−22.242	−19.778	−19.973	−19.880	−19.892	−28.900
$(CH_3)_4Si$	−37.861	−37.876	−38.572	−38.490	−38.479	−55.700
C_5H_6S (2-methyl thiophene)	20.236	22.340	21.425	21.459	21.439	20.000
C_5H_7N (N-methyl pyrrole)	27.932	25.458	25.869	25.790	25.801	24.600
$C_5H_{10}O$ (tetrahydropyran)	−43.172	−43.290	−43.991	−44.127	−44.111	−53.400
$(CH_3CH_2)_2C{=}O$	−52.059	−54.831	−54.433	−54.472	−54.453	−61.600
$C_5H_{10}O_2$ (isopropyl acetate)	−108.711	−108.725	−107.607	−107.713	−107.731	−115.100
$C_5H_{10}S$ (tetrahydrothiopyran)	−2.944	−5.647	−6.531	−6.442	−6.427	−15.200
$C_5H_{11}N$ (piperidine)	−2.386	−1.810	−2.472	−2.565	−2.551	−11.300
$C_5H_{12}O$ (t-butyl methyl ether)	−54.379	−56.707	−56.264	−56.362	−56.348	−67.800
$C_6H_4F_2$ (1,3-difluorobenzene)	−74.603	−74.025	−74.280	−74.292	−74.269	−73.900
$C_6H_4F_2$ (1,4-difluorobenzene)	−69.728	−72.328	−73.406	−73.542	−73.521	−73.300
C_6H_5F (fluorobenzene)	−26.654	−26.339	−26.843	−26.908	−26.887	−27.400
$C_6H_{14}O$ (diisopropyl ether)	−62.529	−63.842	−62.829	−62.933	−62.958	−76.300
PF_5	−360.450	−360.248	−359.971	−360.006	−359.995	−381.100
SF_6	−285.520	−285.026	−284.577	−284.610	−284.594	−291.700
P_4	11.562	11.507	11.519	11.530	11.521	14.100
SO_3	−97.775	−97.915	−97.927	−97.999	−97.990	−94.600
SCl_2	−8.646	−8.605	−8.587	−8.592	−8.590	−4.200
$POCl_3$	−134.265	−133.930	−133.926	−133.933	−133.932	−133.800
PCl_5	−94.178	−93.642	−93.722	−93.756	−93.755	−86.100
Cl_2O_2S	−91.895	−91.213	−91.319	−91.336	−91.325	−84.800
PCl_3	−71.629	−71.638	−71.564	−71.565	−71.566	−69.000
Cl_2S_2	−16.721	−16.524	−16.557	−16.570	−16.572	−4.000
$SiCl_2$ ($^1A_1$)	−38.662	−38.625	−38.576	−38.579	−38.579	−40.300
CF_3Cl	−167.705	−167.675	−167.700	−167.720	−167.707	−169.700
C_2F_6	−312.573	−314.614	−313.948	−313.853	−313.852	−320.900
$^2CF_3$	−113.027	−113.899	−113.913	−113.931	−113.919	−111.800
$^2C_6H_5$ (phenyl radical)	75.764	75.690	75.016	74.910	74.925	80.500
M.D.	1.918	1.825	1.845	1.846	1.845	
M.A.D.	5.372	5.292	5.298	5.299	5.299	

TABLE S3: r^{2}SCAN bond lengths [Å] as function of NWChem grid density.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
H_2	0.742	0.742	0.742	0.742	0.742	0.741
Li_2	2.764	2.761	2.762	2.762	2.762	2.673
LiH	1.605	1.605	1.605	1.605	1.605	1.595
LiF	1.574	1.574	1.573	1.574	1.574	1.564
LiCl	2.028	2.029	2.029	2.029	2.029	2.021
LiO	1.696	1.696	1.696	1.696	1.696	1.688
Be_2	2.486	2.489	2.488	2.489	2.489	2.440
BeH	1.357	1.357	1.357	1.357	1.357	1.343
BeF	1.374	1.374	1.374	1.374	1.374	1.361
BeO	1.335	1.335	1.335	1.335	1.335	1.331
BeS	1.749	1.749	1.749	1.749	1.749	1.742
B_2	1.618	1.618	1.618	1.618	1.618	1.590
BH	1.242	1.242	1.242	1.242	1.242	1.232
BF	1.267	1.267	1.267	1.267	1.267	1.263
BF_3	1.314	1.314	1.314	1.314	1.314	1.313
BCl	1.725	1.724	1.724	1.724	1.724	1.715
BCl_3	1.742	1.742	1.742	1.742	1.742	1.742
BN	1.321	1.321	1.321	1.321	1.321	1.281
BO	1.206	1.206	1.206	1.206	1.206	1.204
BS	1.612	1.612	1.612	1.612	1.612	1.609
C_2	1.250	1.249	1.249	1.249	1.249	1.242
CH	1.126	1.126	1.126	1.126	1.126	1.120
CH_4	1.088	1.088	1.088	1.088	1.088	1.087
CF	1.278	1.278	1.278	1.278	1.278	1.272
CF_4	1.325	1.325	1.325	1.325	1.325	1.323
CCl	1.654	1.654	1.654	1.654	1.654	1.645
CCl_4	1.774	1.774	1.774	1.774	1.774	1.767
CN	1.164	1.164	1.165	1.165	1.165	1.172
CO	1.128	1.127	1.127	1.127	1.127	1.128
CO^+	1.112	1.112	1.112	1.112	1.112	1.115
CO_2	1.162	1.162	1.162	1.162	1.162	1.160
CP	1.555	1.555	1.555	1.555	1.555	1.562
CS	1.536	1.536	1.536	1.536	1.536	1.535
CS_2	1.553	1.552	1.552	1.552	1.552	1.553
N_2	1.093	1.093	1.093	1.093	1.093	1.098
N_2^+	1.107	1.106	1.106	1.106	1.106	1.116
NH	1.041	1.041	1.041	1.041	1.041	1.036
NH^+	1.078	1.078	1.078	1.078	1.078	1.070
NF	1.320	1.319	1.319	1.319	1.319	1.317
NCl	1.616	1.616	1.616	1.616	1.616	1.611
NO	1.148	1.148	1.148	1.148	1.148	1.151
NO^+	1.059	1.059	1.059	1.059	1.059	1.063
NS	1.494	1.494	1.494	1.494	1.494	1.494
O_2	1.207	1.207	1.207	1.207	1.207	1.208
O_2^+	1.109	1.109	1.109	1.109	1.109	1.116
OH	0.973	0.973	0.973	0.973	0.973	0.970
OH^+	1.035	1.035	1.035	1.035	1.035	1.029
OF	1.350	1.350	1.350	1.350	1.350	1.358
F_2	1.399	1.399	1.399	1.399	1.399	1.412
F_2^+	1.297	1.298	1.298	1.298	1.298	1.322
HF	0.921	0.921	0.921	0.921	0.921	0.917
HF^+	1.010	1.010	1.010	1.010	1.010	1.001
Na_2	3.143	3.142	3.142	3.142	3.142	3.079
NaH	1.895	1.898	1.898	1.898	1.898	1.887
NaF	1.926	1.926	1.926	1.926	1.926	1.926
NaCl	2.365	2.365	2.365	2.365	2.365	2.361
NaO	2.054	2.054	2.056	2.056	2.056	2.052
MgH	1.744	1.745	1.745	1.745	1.745	1.730
MgF	1.765	1.766	1.766	1.766	1.766	1.750
MgCl	2.211	2.212	2.212	2.212	2.212	2.196
MgO	1.737	1.736	1.737	1.736	1.736	1.748
Al_2	2.471	2.471	2.471	2.471	2.471	2.466

TABLE S3: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
AlH	1.661	1.662	1.661	1.661	1.661	1.648
AlF	1.664	1.664	1.664	1.664	1.664	1.654
AlCl	2.145	2.145	2.145	2.145	2.145	2.130
AlO	1.619	1.619	1.619	1.619	1.619	1.618
AlS	2.031	2.031	2.031	2.031	2.031	2.029
Si_2	2.152	2.152	2.152	2.152	2.152	2.246
SiH	1.529	1.530	1.530	1.530	1.530	1.520
SiH_4	1.484	1.483	1.483	1.482	1.482	1.480
SiF	1.613	1.613	1.613	1.613	1.613	1.601
SiF_4	1.564	1.564	1.564	1.564	1.564	1.553
SiCl	2.070	2.070	2.070	2.070	2.070	2.058
$SiCl_4$	2.025	2.025	2.025	2.025	2.025	2.019
SiN	1.569	1.569	1.569	1.569	1.569	1.572
SiO	1.515	1.515	1.515	1.515	1.515	1.510
SiS	1.937	1.937	1.937	1.937	1.937	1.929
P_2	1.891	1.891	1.891	1.891	1.891	1.893
P_4	2.190	2.191	2.190	2.190	2.190	2.210
PH	1.427	1.427	1.427	1.427	1.427	1.421
PF	1.598	1.599	1.599	1.599	1.599	1.589
PCl	2.019	2.019	2.019	2.019	2.019	2.015
PN	1.487	1.487	1.487	1.487	1.487	1.491
PO	1.482	1.482	1.482	1.482	1.482	1.476
S_2	1.896	1.896	1.896	1.896	1.896	1.889
SH	1.345	1.345	1.345	1.345	1.345	1.341
SF	1.605	1.605	1.605	1.605	1.605	1.601
SF_6	1.576	1.576	1.576	1.576	1.576	1.561
SO	1.490	1.490	1.490	1.490	1.490	1.481
SO_3	1.429	1.429	1.429	1.429	1.429	1.420
Cl_2	1.996	1.996	1.996	1.996	1.996	1.988
Cl_2^+	1.898	1.898	1.898	1.898	1.898	1.891
HCl	1.279	1.279	1.279	1.279	1.279	1.275
HCl^+	1.321	1.321	1.321	1.321	1.321	1.315
ClF	1.636	1.636	1.636	1.636	1.636	1.628
ClO	1.575	1.575	1.575	1.575	1.575	1.570
M.D.	0.005	0.005	0.005	0.005	0.005	
M.A.D.	0.010	0.010	0.010	0.010	0.010	

TABLE S4: r^{2}SCAN-L bond lengths [Å] as in preceding Table.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
H_2	0.742	0.742	0.742	0.742	0.742	0.741
Li_2	2.728	2.728	2.729	2.729	2.729	2.673
LiH	1.595	1.595	1.595	1.595	1.595	1.595
LiF	1.569	1.569	1.569	1.569	1.569	1.564
LiCl	2.016	2.016	2.016	2.016	2.016	2.021
LiO	1.691	1.690	1.691	1.691	1.691	1.688
Be_2	2.401	2.395	2.395	2.395	2.395	2.440
BeH	1.349	1.349	1.349	1.349	1.349	1.343
BeF	1.373	1.373	1.373	1.373	1.373	1.361
BeO	1.337	1.336	1.336	1.336	1.336	1.331
BeS	1.744	1.744	1.744	1.744	1.744	1.742
B_2	1.612	1.609	1.609	1.609	1.609	1.590
BH	1.240	1.240	1.240	1.240	1.240	1.232
BF	1.270	1.270	1.270	1.270	1.270	1.263
BF_3	1.318	1.318	1.318	1.318	1.318	1.313
BCl	1.723	1.723	1.722	1.722	1.722	1.715
BCl_3	1.741	1.740	1.740	1.740	1.740	1.742
BN	1.323	1.323	1.323	1.323	1.323	1.281
BO	1.208	1.209	1.209	1.209	1.209	1.204
BS	1.610	1.610	1.610	1.610	1.610	1.609
C_2	1.394	1.394	1.394	1.394	1.394	1.242
CH	1.125	1.125	1.125	1.125	1.125	1.120
CH_4	1.088	1.088	1.088	1.088	1.088	1.087
CF	1.286	1.285	1.285	1.285	1.285	1.272
CF_4	1.333	1.333	1.333	1.333	1.333	1.323
CCl	1.658	1.657	1.657	1.657	1.657	1.645
CCl_4	1.778	1.778	1.778	1.778	1.778	1.767
CN	1.169	1.169	1.169	1.169	1.169	1.172
CO	1.132	1.132	1.132	1.132	1.132	1.128
CO^+	1.116	1.116	1.116	1.116	1.116	1.115
CO_2	1.167	1.167	1.167	1.167	1.167	1.160
CP	1.556	1.556	1.556	1.556	1.556	1.562
CS	1.539	1.539	1.539	1.539	1.539	1.535
CS_2	1.554	1.554	1.554	1.554	1.554	1.553
N_2	1.099	1.099	1.099	1.099	1.099	1.098
N_2^+	1.110	1.110	1.110	1.110	1.110	1.116
NH	1.044	1.043	1.043	1.043	1.043	1.036
NH^+	1.080	1.080	1.080	1.080	1.080	1.070
NF	1.330	1.330	1.330	1.330	1.330	1.317
NCl	1.623	1.622	1.622	1.622	1.622	1.611
NO	1.155	1.155	1.155	1.155	1.155	1.151
NO^+	1.066	1.066	1.066	1.066	1.066	1.063
NS	1.501	1.500	1.500	1.500	1.500	1.494
O_2	1.218	1.218	1.218	1.218	1.218	1.208
O_2^+	1.119	1.119	1.119	1.119	1.119	1.116
OH	0.975	0.975	0.975	0.975	0.975	0.970
OH^+	1.038	1.038	1.038	1.038	1.038	1.029
OF	1.364	1.364	1.364	1.364	1.364	1.358
F_2	1.415	1.415	1.415	1.415	1.415	1.412
F_2^+	1.318	1.318	1.318	1.318	1.318	1.322
HF	0.924	0.924	0.924	0.924	0.924	0.917
HF^+	1.011	1.011	1.011	1.011	1.011	1.001
Na_2	3.121	3.120	3.120	3.120	3.120	3.079
NaH	1.887	1.887	1.887	1.887	1.887	1.887
NaF	1.928	1.926	1.926	1.926	1.926	1.926
NaCl	2.357	2.357	2.357	2.357	2.357	2.361
NaO	2.052	2.052	2.053	2.053	2.053	2.052
MgH	1.734	1.735	1.735	1.735	1.735	1.730
MgF	1.765	1.766	1.766	1.766	1.766	1.750
MgCl	2.204	2.204	2.204	2.204	2.204	2.196
MgO	1.738	1.738	1.737	1.737	1.737	1.748
Al_2	2.463	2.462	2.462	2.462	2.462	2.466

TABLE S4: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
AlH	1.656	1.657	1.656	1.656	1.656	1.648
AlF	1.666	1.666	1.666	1.666	1.666	1.654
AlCl	2.140	2.140	2.140	2.140	2.140	2.130
AlO	1.620	1.619	1.619	1.619	1.619	1.618
AlS	2.029	2.028	2.028	2.028	2.028	2.029
Si_2	2.263	2.263	2.263	2.263	2.263	2.246
SiH	1.524	1.524	1.524	1.524	1.524	1.520
SiH_4	1.480	1.479	1.479	1.479	1.479	1.480
SiF	1.617	1.617	1.617	1.617	1.617	1.601
SiF_4	1.567	1.567	1.567	1.567	1.567	1.553
SiCl	2.067	2.067	2.067	2.067	2.067	2.058
$SiCl_4$	2.024	2.024	2.024	2.024	2.024	2.019
SiN	1.570	1.570	1.570	1.570	1.570	1.572
SiO	1.519	1.519	1.519	1.519	1.519	1.510
SiS	1.937	1.937	1.937	1.937	1.937	1.929
P_2	1.892	1.892	1.892	1.892	1.892	1.893
P_4	2.193	2.193	2.193	2.193	2.193	2.210
PH	1.425	1.425	1.424	1.424	1.424	1.421
PF	1.606	1.607	1.607	1.607	1.607	1.589
PCl	2.021	2.021	2.021	2.021	2.021	2.015
PN	1.492	1.492	1.492	1.492	1.492	1.491
PO	1.488	1.488	1.488	1.488	1.488	1.476
S_2	1.900	1.900	1.900	1.900	1.900	1.889
SH	1.342	1.342	1.342	1.342	1.342	1.341
SF	1.617	1.617	1.617	1.617	1.617	1.601
SF_6	1.589	1.589	1.589	1.589	1.588	1.561
SO	1.499	1.499	1.499	1.499	1.499	1.481
SO_3	1.438	1.438	1.438	1.438	1.438	1.420
Cl_2	2.006	2.005	2.005	2.005	2.005	1.988
Cl_2^+	1.908	1.908	1.908	1.908	1.908	1.891
HCl	1.277	1.277	1.277	1.277	1.277	1.275
HCl^+	1.319	1.319	1.319	1.319	1.319	1.315
ClF	1.651	1.651	1.651	1.651	1.651	1.628
ClO	1.588	1.587	1.587	1.587	1.587	1.570
M.D.	0.008	0.008	0.008	0.008	0.008	
M.A.D.	0.011	0.011	0.011	0.011	0.011	

TABLE S5: r^{2}SCAN harmonic vibrational frequencies [cm^{-1}] as function of NWChem grid density.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
H_2	4434.420	4429.000	4429.780	4429.670	4429.670	4401.200
Li_2	333.880	332.890	333.320	332.370	332.510	351.400
LiH	1390.860	1382.190	1392.260	1394.280	1395.470	1405.700
LiF	888.110	905.170	897.820	904.770	902.250	910.600
LiCl	648.750	642.780	643.690	642.660	642.490	643.000
LiO	820.600	808.730	813.440	810.720	809.870	814.600
LiNa	247.550	244.270	245.500	246.330	246.200	256.800
Be_2	328.310	326.760	327.350	327.200	327.150	267.900
BeH	2006.420	2017.610	2014.180	2009.730	2010.780	2060.800
BeH^+	2192.550	2201.980	2201.390	2203.030	2203.110	2221.700
BeF	1233.950	1226.040	1222.060	1222.540	1224.400	1247.400
BeCl	813.660	818.490	816.740	816.440	816.460	846.700
BeO	1511.470	1508.930	1508.230	1508.310	1508.740	1487.300
BeS	1011.030	1009.280	1007.820	1008.220	1007.990	997.900
B_2	1013.660	1017.520	1010.540	1012.940	1012.940	1051.300
BH	2311.530	2308.950	2303.790	2301.010	2301.450	2366.900
BF	1401.890	1399.820	1398.310	1398.460	1398.720	1402.100
BCl	823.740	825.480	826.290	826.560	826.520	840.300
BN	1571.930	1569.980	1570.340	1570.170	1570.010	1514.600
BO	1892.940	1895.790	1896.250	1896.330	1896.390	1885.700
BS	1196.440	1194.770	1195.610	1195.470	1195.510	1180.200
C_2	1886.130	1892.790	1890.120	1891.110	1891.600	1854.700
CH	2804.930	2807.290	2807.420	2803.920	2803.830	2858.500
CF	1290.990	1297.580	1297.060	1297.420	1297.490	1308.100
CN	2155.020	2149.480	2149.500	2149.610	2149.590	2068.600
CO	2192.450	2195.650	2194.900	2195.550	2195.160	2169.800
CO^+	2276.670	2277.870	2277.930	2277.960	2277.850	2214.200
CP	1281.100	1285.620	1288.180	1286.420	1286.590	1239.700
CS	1305.440	1303.910	1304.040	1304.750	1304.550	1285.200
N_2	2429.490	2430.610	2432.640	2432.680	2432.760	2358.600
N_2^+	2319.480	2327.810	2327.300	2326.820	2326.750	2207.000
NH	3257.570	3242.170	3249.950	3246.500	3246.440	3282.300
NF	1147.300	1171.670	1171.370	1171.320	1171.310	1141.400
NCl	832.860	835.830	836.870	836.470	836.420	828.000
NO	1957.380	1959.050	1959.420	1959.480	1959.480	1904.200
NO^+	2458.760	2456.780	2456.150	2456.140	2456.150	2376.400
NS	1256.740	1256.110	1253.960	1254.450	1254.480	1218.700
O_2	1629.380	1625.260	1624.450	1624.960	1624.980	1580.200
O_2^+	2028.500	2026.660	2025.910	2026.490	2026.550	1904.800
OH	3721.000	3717.900	3717.590	3718.310	3718.280	3737.800
OH^+	3058.640	3060.440	3061.330	3060.890	3060.970	3113.400
F_2	1052.000	1046.970	1048.290	1048.270	1048.450	916.600
F_2^+	1216.600	1219.390	1219.780	1219.830	1219.830	1073.300
HF	4097.590	4093.600	4093.330	4093.340	4093.320	4138.300
HF^+	3001.810	3029.230	3024.180	3024.750	3024.740	3090.500
Na_2	155.730	155.510	155.280	155.290	155.310	159.100
NaH	1187.380	1172.340	1175.580	1167.880	1163.940	1172.200
NaF	532.770	535.970	539.460	539.360	538.900	535.700
NaO	496.710	491.750	487.620	488.060	487.240	492.300
MgH	1421.990	1451.580	1466.010	1461.590	1460.760	1495.200
MgH^+	1747.510	1738.650	1723.990	1720.880	1717.510	1699.100
MgO	840.650	834.490	837.360	837.420	836.580	784.800
MgS	551.550	551.680	550.640	550.230	550.870	528.700
Al_2	355.930	356.260	355.860	355.770	355.850	350.000
AlH	1628.910	1645.320	1651.400	1646.500	1648.010	1682.600
AlF	795.990	784.540	785.710	788.750	787.480	802.300
AlCl	476.240	475.620	475.220	475.870	475.640	481.300
AlO	993.280	994.350	993.560	992.270	992.590	979.200
AlS	631.070	630.890	630.600	630.550	630.660	617.100
Si_2	564.420	564.830	563.910	564.410	564.210	511.000
SiH	1957.670	2022.280	2028.960	2020.550	2023.130	2041.800
SiH^+	2050.080	2127.260	2127.340	2119.640	2121.250	2157.200

TABLE S5: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
SiF	845.990	843.640	845.990	847.320	846.540	857.200
SiCl	529.700	529.110	529.240	529.270	529.130	535.600
SiN	1175.850	1185.040	1180.700	1179.680	1180.800	1151.400
SiO	1257.740	1250.070	1244.590	1247.890	1247.210	1241.500
SiS	753.770	753.420	753.330	753.330	753.470	749.600
P_2	813.710	813.130	813.590	813.930	813.550	780.800
P_2^+	709.250	707.770	707.720	707.910	707.990	672.200
PH	2327.790	2361.610	2372.030	2367.880	2367.510	2365.200
PF	845.170	844.180	846.370	846.900	846.490	846.800
PCl	550.240	550.140	550.280	550.120	550.190	551.400
PN	1386.950	1389.910	1392.240	1390.710	1390.530	1337.200
PO	1252.700	1252.000	1249.480	1250.590	1250.690	1233.300
S_2	732.600	732.580	732.450	732.630	732.420	725.600
SO	1157.620	1157.930	1158.300	1159.280	1158.950	1149.200
Cl_2	555.460	555.340	555.440	555.490	555.410	559.700
Cl_2^+	649.610	649.260	649.280	649.260	649.320	645.600
HCl	2967.070	2974.720	2978.080	2981.860	2980.000	2990.900
HCl^+	2662.340	2649.650	2651.350	2643.920	2645.020	2673.700
ClF	794.690	791.060	791.330	791.240	791.290	786.100
ClO	871.700	872.720	872.110	872.510	872.360	853.800
M.D.	9.007	11.609	11.805	11.349	11.271	
M.A.D.	34.198	31.075	30.622	30.900	30.874	

TABLE S6: r^{2}SCAN-L harmonic vibrational frequencies [cm^{-1}] as in preceding Table.

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
H_2	4436.680	4432.060	4432.740	4433.000	4433.000	4401.200
Li_2	339.790	339.650	339.320	338.500	338.410	351.400
LiH	1398.290	1395.100	1404.430	1398.390	1402.600	1405.700
LiF	885.650	901.170	895.550	900.090	899.630	910.600
LiCl	653.230	645.980	647.090	647.690	646.750	643.000
LiO	814.910	802.330	808.820	805.460	805.540	814.600
LiNa	251.350	249.410	249.310	249.040	249.240	256.800
Be_2	379.040	376.900	379.160	378.910	378.880	267.900
BeH	2026.360	2037.010	2033.330	2032.610	2034.870	2060.800
BeH^+	2198.050	2206.270	2202.690	2204.430	2205.920	2221.700
BeF	1228.660	1219.740	1216.800	1216.820	1218.750	1247.400
BeCl	821.200	826.640	828.850	828.520	828.550	846.700
BeO	1489.860	1486.170	1485.340	1485.150	1485.920	1487.300
BeS	1005.170	1001.840	1001.700	1002.210	1001.860	997.900
B_2	1020.720	1025.680	1027.330	1026.000	1026.870	1051.300
BH	2312.920	2323.420	2312.640	2311.730	2311.850	2366.900
BF	1380.760	1375.250	1374.580	1374.720	1375.070	1402.100
BCl	821.040	820.310	821.860	822.020	822.050	840.300
BN	1549.900	1545.740	1547.340	1547.060	1546.890	1514.600
BO	1846.020	1867.060	1866.990	1866.830	1866.970	1885.700
BS	1186.410	1184.940	1184.980	1185.040	1185.050	1180.200
C_2	1867.880	1875.720	1872.900	1873.680	1874.040	1854.700
CH	2801.500	2798.540	2805.970	2802.620	2802.510	2858.500
CF	1251.800	1257.710	1256.900	1257.130	1257.210	1308.100
CN	2114.040	2113.640	2113.140	2113.030	2112.910	2068.600
CO	2142.970	2145.080	2144.830	2145.550	2145.240	2169.800
CO^+	2227.510	2227.900	2227.020	2226.890	2226.900	2214.200
CP	1264.870	1270.990	1270.910	1269.350	1269.880	1239.700
CS	1280.230	1278.990	1278.630	1279.880	1279.660	1285.200
N_2	2366.240	2372.020	2372.460	2371.770	2371.900	2358.600
N_2^+	2276.100	2280.010	2282.060	2282.720	2282.480	2207.000
NH	3217.790	3215.400	3212.930	3217.630	3217.410	3282.300
NF	1125.820	1123.840	1122.690	1122.990	1123.030	1141.400
NCl	818.470	822.430	823.160	823.160	822.920	828.000
NO	1892.360	1892.490	1893.400	1893.370	1893.340	1904.200
NO^+	2383.230	2380.500	2379.550	2379.660	2379.640	2376.400
NS	1224.550	1223.050	1219.760	1220.840	1220.630	1218.700
O_2	1552.570	1552.800	1552.180	1552.320	1552.260	1580.200
O_2^+	1935.160	1933.440	1932.910	1934.210	1933.030	1904.800
OH	3691.780	3690.140	3689.540	3689.780	3689.690	3737.800
OH^+	3022.280	3015.470	3024.060	3023.950	3023.670	3113.400
F_2	1012.340	1003.590	1004.640	1007.200	1004.910	916.600
F_2^+	1146.440	1155.510	1154.350	1154.360	1153.250	1073.300
HF	4063.670	4048.580	4047.960	4047.570	4047.550	4138.300
HF^+	2977.240	3004.110	2999.540	3000.160	3000.180	3090.500
Na_2	156.350	157.190	156.980	156.890	156.770	159.100
NaH	1189.320	1178.150	1181.930	1170.470	1169.000	1172.200
NaF	526.820	530.740	533.600	533.810	533.250	535.700
NaO	491.800	487.800	483.840	483.340	483.070	492.300
MgH	1446.640	1470.260	1483.680	1480.390	1476.910	1495.200
MgH^+	1746.080	1740.080	1722.890	1721.290	1718.090	1699.100
MgO	825.900	820.340	823.570	823.410	822.770	784.800
MgS	544.740	545.370	544.060	543.510	543.950	528.700
Al_2	354.930	354.860	354.690	354.350	354.480	350.000
AlH	1626.020	1646.840	1655.750	1651.230	1651.500	1682.600
AlF	783.820	772.630	773.250	776.710	775.420	802.300
AlCl	473.650	473.060	472.880	473.410	473.140	481.300
AlO	989.290	986.720	986.800	985.140	985.520	979.200
AlS	625.040	625.990	626.000	625.830	625.960	617.100
Si_2	501.070	499.690	499.760	499.330	499.440	511.000
SiH	1976.580	2033.680	2039.310	2030.650	2031.970	2041.800
SiH^+	2057.630	2120.100	2124.580	2110.970	2113.480	2157.200

TABLE S6: (continued)

System	COARSE	MEDIUM	FINE	XFINE	HUGE	Exptl.
SiF	828.900	827.720	829.640	830.920	830.270	857.200
SiCl	525.210	524.350	524.290	524.410	524.290	535.600
SiN	1164.640	1172.020	1167.250	1166.460	1167.290	1151.400
SiO	1228.010	1221.030	1217.000	1219.920	1219.180	1241.500
SiS	742.680	741.770	741.610	741.630	741.740	749.600
P_2	798.560	798.070	798.530	798.720	798.410	780.800
P_2^+	695.180	693.900	693.580	693.660	694.090	672.200
PH	2314.980	2356.000	2364.660	2363.180	2361.770	2365.200
PF	819.440	816.970	820.690	821.170	820.420	846.800
PCl	538.780	538.890	539.250	539.060	539.130	551.400
PN	1356.000	1357.270	1359.760	1357.510	1358.000	1337.200
PO	1214.100	1218.140	1215.000	1214.130	1214.930	1233.300
S_2	714.170	713.810	711.890	713.940	713.870	725.600
SO	1117.830	1116.840	1115.160	1115.800	1115.970	1149.200
Cl_2	536.020	535.780	535.850	535.880	535.880	559.700
Cl_2^+	629.950	629.840	629.930	629.910	629.920	645.600
HCl	2955.810	2965.470	2956.990	2965.120	2963.660	2990.900
HCl^+	2638.650	2628.930	2634.220	2630.240	2630.560	2673.700
ClF	761.700	758.450	758.670	758.600	758.410	786.100
ClO	844.950	844.780	843.540	843.630	843.530	853.800
M.D.	−9.472	−6.984	−6.797	−7.221	−7.266	
M.A.D.	29.258	26.166	25.619	25.748	25.624	

TABLE S7: Equilibrium lattice constants (Å) obtained in VASP.

System	SCAN	SCAN-L	r^{2}SCAN	r^{2}SCAN-L	Exptl.
C	3.557	3.574	3.564	3.571	3.553
Si	5.428	5.420	5.440	5.427	5.421
Ge	5.685	5.701	5.681	5.705	5.644
Sn	6.557	6.568	6.565	6.580	6.477
SiC	4.352	4.362	4.356	4.356	4.346
BN	3.607	3.615	3.614	3.620	3.592
BP	4.523	4.529	4.533	4.538	4.525
AlN	4.362	4.369	4.368	4.366	4.368
AlP	5.465	5.449	5.473	5.459	5.451
AlAs	5.671	5.653	5.677	5.675	5.649
GaN	4.527	4.544	4.527	4.547	4.520
GaP	5.462	5.482	5.467	5.477	5.439
GaAs	5.665	5.681	5.672	5.694	5.640
InP	5.936	5.947	5.947	5.941	5.858
InAs	6.122	6.122	6.132	6.141	6.047
InSb	6.546	6.544	6.569	6.577	6.468
LiH	4.000	3.971	4.012	3.988	3.979
LiF	3.978	4.013	3.995	4.005	3.972
LiCl	5.094	5.061	5.111	5.073	5.070
NaF	4.480	4.506	4.503	4.511	4.582
NaCl	5.520	5.488	5.546	5.509	5.569
MgO	4.187	4.205	4.197	4.197	4.189
Li	3.469	3.435	3.479	3.430	3.443
Na	4.181	4.145	4.200	4.139	4.214
K	5.305	5.262	5.351	5.282	5.212
Rb	5.707	5.631	5.752	5.694	5.577
Cs	6.225	6.123	6.262	6.174	6.039
Ca	5.547	5.490	5.575	5.503	5.556
Ba	5.052	5.038	5.077	5.051	5.002
Sr	6.087	6.308	6.106	6.045	6.040
Al	4.006	4.002	3.988	3.973	4.018
Fe	2.840	2.794	2.865	2.830	2.853
Co	3.508	3.488	3.513	3.508	3.524
Ni	3.462	3.472	3.479	3.497	3.508
Sc	3.245	3.219	3.260	3.228	3.270
Y	3.614	3.602	3.623	3.602	3.594
Ti	2.882	2.873	2.887	2.878	2.915
Zr	3.206	3.211	3.215	3.216	3.198
Hf	3.117	3.143	3.141	3.151	3.151
V	2.953	2.960	2.965	2.965	3.021
Nb	3.311	3.317	3.321	3.324	3.294
Ta	3.272	3.289	3.290	3.301	3.299
Mo	3.136	3.138	3.144	3.148	3.141
W	3.139	3.154	3.156	3.166	3.160
Tc	2.706	2.712	2.716	2.723	2.716
Re	2.727	2.746	2.750	2.760	2.744
Ru	2.646	2.670	2.672	2.683	2.669
Os	2.684	2.706	2.708	2.722	2.699
Rh	3.778	3.800	3.804	3.824	3.794
Ir	3.788	3.845	3.852	3.876	3.831
Pd	3.894	3.913	3.912	3.938	3.876
Pt	3.897	3.942	3.943	3.975	3.913
Cu	3.568	3.562	3.583	3.609	3.595
Ag	4.084	4.101	4.107	4.138	4.062
Au	4.089	4.126	4.127	4.167	4.062
M.D.	0.009	0.012	0.026	0.020	
M.A.D.	0.033	0.037	0.037	0.039	

TABLE S8: Bulk moduli (GPa) obtained in VASP.

System	SCAN	SCAN-L	r^{2}SCAN	r^{2}SCAN-L	Exptl.
C	458.647	433.253	449.405	433.982	454.700
Si	99.141	96.940	97.292	95.184	101.300
Ge	71.514	66.061	73.052	67.964	79.400
Sn	41.858	39.870	43.523	41.064	42.800
SiC	227.351	221.446	226.621	218.232	229.100
BN	393.110	382.392	390.180	377.997	410.200
BP	173.476	162.174	169.686	164.715	168.000
AlN	213.130	209.042	212.552	208.034	206.000
AlP	91.319	89.954	91.074	89.419	87.400
AlAs	76.847	76.127	76.333	73.893	75.000
GaN	212.015	196.281	211.429	198.258	213.000
GaP	91.875	85.149	90.426	87.139	89.600
GaAs	74.845	70.373	73.771	69.835	76.700
InP	70.816	66.223	70.264	67.903	72.000
InAs	58.762	56.443	58.918	55.701	58.600
InSb	43.618	42.809	44.018	42.034	46.100
LiH	36.266	39.524	36.277	38.305	40.100
LiF	80.042	74.731	78.326	75.355	76.300
LiCl	36.063	40.657	35.068	37.619	38.700
NaF	62.750	64.691	60.090	59.092	53.100
NaCl	30.225	29.728	29.008	30.547	27.600
MgO	172.236	167.319	170.456	167.913	169.800
Li	13.683	16.198	13.129	14.571	13.100
Na	8.027	7.962	7.928	8.848	7.900
K	3.446	3.787	3.413	3.833	3.800
Rb	2.876	2.705	2.630	2.817	3.600
Cs	2.038	2.059	2.007	2.143	2.300
Ca	18.082	19.307	17.751	19.055	15.900
Ba	8.679	9.092	8.543	8.958	10.600
Sr	11.424	−4.438	11.237	11.957	12.000
Al	77.521	95.268	91.946	89.976	77.100
Ni	231.672	230.889	216.919	198.967	192.500
V	202.913	198.111	200.584	197.016	165.800
Nb	181.442	178.156	178.188	175.169	173.200
Ta	214.572	208.929	209.993	206.779	202.700
Mo	284.929	278.934	281.488	268.695	276.200
W	340.499	328.189	330.480	318.293	327.500
Rh	294.753	272.414	281.261	255.753	277.100
Ir	405.332	372.180	379.091	342.250	362.200
Pd	195.076	174.190	186.121	167.042	187.200
Pt	293.847	262.731	273.050	241.313	285.500
Cu	160.577	168.658	160.644	148.838	144.300
Ag	110.292	103.323	103.511	91.974	105.700
Au	167.405	149.315	153.691	133.303	182.000
M.D.	4.575	−1.240	1.311	−5.363	
M.A.D.	7.358	8.821	5.966	8.988	

TABLE S9: Cohesive energies (eV/atom) obtained in VASP.

System	SCAN	SCAN-L	r^{2}SCAN	r^{2}SCAN-L	Exptl.
C	7.495	7.361	7.458	7.353	7.550
Si	4.712	4.550	4.675	4.500	4.680
Ge	3.981	3.663	3.891	3.527	3.890
Sn	3.430	3.216	3.295	3.039	3.160
SiC	6.444	6.274	6.428	6.228	6.480
BN	6.832	6.771	6.785	6.709	6.760
BP	5.325	5.202	5.279	5.149	5.140
AlN	5.818	5.739	5.809	5.712	5.850
AlP	4.267	4.178	4.249	4.127	4.320
AlAs	3.897	3.737	3.867	3.673	3.820
GaN	4.466	4.327	4.464	4.308	4.550
GaP	3.661	3.460	3.641	3.439	3.610
GaAs	3.373	3.125	3.328	3.059	3.340
InP	3.238	3.092	3.244	3.100	3.470
InAs	3.036	2.835	3.026	2.807	3.080
InSb	2.812	2.638	2.729	2.570	2.810
LiH	2.456	2.432	2.430	2.418	2.490
LiF	4.414	4.256	4.402	4.284	4.460
LiCl	3.505	3.413	3.477	3.409	3.590
NaF	3.987	3.840	3.989	3.871	3.970
NaCl	3.271	3.178	3.259	3.182	3.340
MgO	5.246	5.157	5.246	5.129	5.200
Li	1.606	1.603	1.590	1.606	1.670
Na	1.055	1.028	1.040	1.022	1.120
K	0.848	0.813	0.839	0.820	0.940
Rb	0.753	0.718	0.734	0.693	0.860
Cs	0.669	0.603	0.657	0.637	0.810
Ca	1.913	2.009	1.917	1.987	1.870
Ba	1.820	1.857	1.817	1.828	1.910
Sr	1.803	1.737	1.785	1.723	1.730
Al	3.605	3.497	3.608	3.427	3.430
Fe	4.575	4.607	4.635	4.487	4.300
Co	4.793	4.946	4.871	4.434	4.420
Ni	4.439	4.426	4.642	4.311	4.480
Sc	4.064	4.004	4.017	3.879	3.930
Y	4.076	3.880	4.013	3.770	4.390
Ti	5.046	4.855	5.057	4.924	4.880
Zr	6.016	5.850	5.934	5.726	6.270
Hf	6.500	6.166	6.435	6.054	6.460
V	4.708	5.156	4.660	4.813	5.350
Nb	6.568	6.632	6.359	6.168	7.600
Ta	8.609	7.994	8.251	7.729	8.130
Mo	5.916	6.192	5.690	5.623	6.860
W	9.007	8.227	9.036	7.620	8.940
Tc	6.552	6.712	6.336	6.222	6.880
Re	8.533	8.014	7.512	7.153	8.050
Ru	6.481	6.544	6.337	5.994	6.770
Os	8.869	8.204	8.072	7.536	8.200
Rh	5.448	5.288	5.486	5.288	5.780
Ir	7.596	7.047	7.157	6.581	6.990
Pd	4.367	4.046	4.165	3.718	3.930
Pt	6.229	5.370	5.716	5.114	5.870
Cu	3.882	3.621	3.857	3.490	3.510
Ag	2.882	2.686	2.874	2.508	2.960
Au	3.555	3.293	3.418	2.950	3.830
M.D.	−0.004	−0.157	−0.094	−0.314	
M.A.D.	0.209	0.212	0.200	0.327	

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