

**Table 1** For each compound the results are given in five lines. They present lattice constant (Å), band gap (eV), position of the CBM (eV), position of the VBM (eV) with respect to the BPE, and the relative size of the stable region with respect to the total area of the stability triangle (in %), respectively.

PBE refers to the calculated results using the PBE functional.

Interp. HSE means that the HSE results of the corresponding binary oxides are used to calculate the values.  $PBE^{aver.}$  results are the average over the four considered configurations of  $(X_{0.5}Y_{0.5})_2O_3$ .

The stability triangle is only plotted based on the PBE calculated results, therefore there is no data in Table 1 for the HSE interpolated relative size of the stable region with respect to the total area of the stability triangle.

The few cases in which the calculations failed to converge, are denoted by a "×".

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
BiCe	11.341	11.358	11.307	11.23	11.311	11.338	11.297	11.311	11.252	11.264
	2.574	4.882	2.284	2.630	2.680	2.480	2.519	4.311	2.746	3.740
	1.170	2.221	-3.696	1.415	1.369	1.300	0.097	2.057	1.645	1.893
	-1.404	-2.662	-5.980	-1.215	-1.312	-1.181	-2.422	-2.255	-1.102	-1.848
	8.771		19.431	19.463	19.509	19.640	19.511		30.309	
BiDy	10.811	10.812	10.946	10.947	10.959	10.942	10.949	10.947	11.073	11.082
	2.582	5.214	2.418	2.537	2.499	2.532	2.497	4.533	2.738	3.851
	1.262	2.294	1.157	1.144	1.141	1.193	1.159	2.106	1.622	1.917
	-1.320	-2.921	-1.261	-1.393	-1.359	-1.339	-1.338	-2.427	-1.117	-1.934
	8.680		19.064	19.318	19.148	19.228	19.189		28.677	
BiEr	10.715	10.704	10.885	10.778	10.895	10.878	10.859	10.875	11.047	11.046
	2.546	5.282	2.406	2.514	2.462	2.510	2.473	4.578	2.719	3.873
	1.236	2.276	1.160	1.143	1.114	1.173	1.148	2.094	1.592	1.911
	-1.310	-3.006	-1.246	-1.372	-1.348	-1.338	-1.326	-2.484	-1.127	-1.962
	4.808		12.589	12.983	12.682	12.727	12.745		26.018	
BiEu	10.902	10.908	10.960	10.961	10.965	10.965	10.963	11.011	11.023	11.114
	2.591	5.180	2.412	2.562	2.535	2.510	2.505	4.510	2.775	3.840
	1.268	2.330	1.204	1.243	1.241	1.173	1.216	2.130	1.704	1.929
	-1.324	-2.851	-1.209	-1.319	-1.294	-1.338	-1.290	-2.381	-1.072	-1.911
	5.337		13.139	13.257	13.194	13.204	13.397		26.707	
BiFe	9.528	9.537	10.013	9.979	10.090	10.557	10.160	10.097	10.663	10.657
	0	0.812	0.001	0	0	0	0.001	1.598	0	2.383
	0.247	1.527	0.426	0.434	0.357	0.419	0.409	1.594	-5.894	1.662
	0.290	0.715	0.426	0.437	0.372	0.457	0.423	-0.004	-5.851	-0.722
	2.401		7.118	12.390	11.982	11.922	10.853		21.443	
BiGa	10.042	9.861	10.371	10.310	10.844	10.557	10.521	10.313	10.824	10.765
	1.624	4.133	2.354	2.247	2.406	2.377	2.346	3.812	1.790	3.491
	0.908	0.826	1.039	0.988	1.059	1.158	1.061	1.127	0.806	1.428
	-0.716	-3.308	-1.316	-1.260	-1.347	-1.220	-1.286	-2.686	-0.985	-2.063
	1.062		13.518	15.429	15.911	15.446	15.076		24.398	
BiGd	10.916	10.915	11.021	11.012	11.019	11.013	11.017	11.016	11.106	11.117
	2.575	5.427	2.427	2.544	2.518	2.540	2.508	4.674	2.729	3.922
	1.232	2.467	1.156	1.181	1.177	1.226	1.185	2.221	1.618	1.975
	-1.344	-2.960	-1.271	-1.364	-1.342	-1.315	-1.323	-2.454	-1.112	-1.947
	5.188		13.005	13.100	13.028	13.074	13.052		26.469	
BiHo	10.754	10.758	10.914	10.917	10.927	10.905	10.916	10.911	11.055	11.064
	2.567	5.257	2.407	2.530	2.483	2.524	2.486	4.561	2.723	3.865
	1.257	2.258	1.155	1.136	1.129	1.187	1.152	2.082	1.604	1.906
	-1.311	-2.999	-1.253	-1.395	-1.355	-1.337	-1.335	-2.480	-1.120	-1.960
	4.886		12.654	12.831	12.727	12.765	12.744		26.066	

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$			$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$	
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
BiIn	10.537	10.533	10.634	10.784	10.826	10.752	10.749	10.761	11.041	10.989
	1.458	2.929	1.921	2.367	2.252	2.200	2.185	3.009	2.426	3.089
	0.436	-0.011	0.892	1.190	1.139	1.060	1.071	0.570	1.386	1.149
	-1.022	-2.939	-1.029	-1.177	-1.114	-1.140	-1.115	-2.440	-1.041	-1.940
	6.918		17.625	18.371	18.117	18.013	18.032		27.911	
BiLa	11.356	11.336	11.323	11.189	11.324	11.333	11.293	11.296	11.254	11.257
	2.652	4.881	2.360	2.696	2.744	2.562	2.591	4.311	2.773	3.740
	1.341	2.165	1.376	1.528	1.458	1.330	1.423	2.020	1.715	1.874
	-1.311	-2.717	-0.984	-1.168	-1.286	-1.232	-1.168	-2.291	-1.059	-1.866
	7.659		18.208	18.692	18.466	18.372	18.435		30.562	
BiLu	10.577	10.575	10.784	10.685	10.805	10.778	10.763	10.789	11.007	11.003
	2.545	5.342	2.391	2.479	2.414	2.469	2.439	4.618	2.696	3.894
	1.267	2.259	1.170	1.107	1.069	1.145	1.123	2.083	1.564	1.906
	-1.279	-3.084	-1.221	-1.372	-1.346	-1.324	-1.316	-2.536	-1.133	-1.988
	5.852		15.189	15.812	15.403	15.458	15.466		28.185	
BiMn	9.983	9.580	10.339	10.059	10.352	10.256	10.252	10.126	10.636	10.672
	0	2.462	0	0	0	0	0	2.698	0	2.934
	0.711	1.393	0.770	0.718	0.680	0.715	0.721	1.505	0.415	1.617
	0.883	-1.070	0.781	0.726	0.692	0.742	0.736	-1.193	0.604	-1.317
	5.523		8.229	15.196	18.252	13.188	13.716		0	
BiPm	11.108	11.108	11.145	11.139	11.131	11.146	11.141	11.144	11.171	11.181
	2.595	5.047	2.361	2.548	2.602	2.524	2.509	4.421	2.747	3.795
	1.213	2.282	1.193	1.280	-3.677	1.285	0.021	2.098	1.645	1.914
	-1.383	-2.765	-1.169	-1.269	-6.278	-1.24	-2.489	-2.323	-1.102	-1.882
	8.705		18.987	19.139	19.01	19.098	19.059		29.928	
BiPr	11.273	11.190	11.261	11.252	11.262	11.262	11.26	11.199	11.229	11.208
	2.607	5.016	2.334	2.602	2.653	2.523	2.528	4.401	2.754	3.785
	1.195	2.285	1.263	1.359	1.342	1.329	1.324	2.100	1.652	1.915
	-1.412	-2.732	-1.072	-1.244	-1.311	-1.195	-1.206	-2.301	-1.103	-1.871
	7.192		18.114	18.278	18.163	18.208	18.191		29.183	
BiSc	10.247	10.241	10.546	10.571	10.619	10.538	10.569	10.566	10.901	10.892
	2.048	5.446	2.230	2.402	2.301	2.293	2.307	4.687	2.472	3.928
	1.508	2.781	1.449	1.379	1.315	1.392	1.384	2.430	1.520	2.080
	-0.540	-2.666	-0.781	-1.024	-0.986	-0.902	-0.924	-2.257	-0.953	-1.849
	3.271		11.164	11.736	11.465	11.508	11.468		24.839	
BiSm	11.053	11.055	11.112	11.099	11.102	11.106	11.105	11.109	11.153	11.163
	2.577	5.065	2.383	2.532	2.547	2.528	2.498	4.433	2.740	3.801
	1.207	2.275	1.146	1.238	1.235	1.265	1.221	2.093	1.635	1.911
	-1.371	-2.791	-1.237	-1.295	-1.312	-1.263	-1.277	-2.341	-1.105	-1.891
	7.861		17.757	17.878	17.761	17.853	17.812		29.837	
BiTb	10.859	10.86	10.984	10.981	10.989	10.975	10.983	10.979	11.091	11.098
	2.565	5.188	2.429	2.539	2.517	2.539	2.506	4.515	2.742	3.842
	1.231	2.296	1.159	1.161	1.160	1.208	1.172	2.107	1.625	1.918
	-1.335	-2.893	-1.271	-1.379	-1.357	-1.332	-1.335	-2.409	-1.118	-1.925
	10.240		20.120	20.400	20.217	20.314	20.263		25.703	
BiTl	10.882	10.879	11.014	11.055	11.068	11.016	11.039	10.992	11.140	11.105
	0.880	1.116	1.138	1.300	1.282	1.286	1.252	1.800	1.928	2.485
	0.202	-1.070	0.281	0.359	0.364	0.403	0.352	-0.137	0.962	0.796
	-0.679	-2.185	-0.858	-0.941	-0.919	-0.883	-0.901	-1.937	-0.967	-1.689

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	10.945		22.365	20.509	20.380	20.116	20.842		26.153	
BiTm	10.660	10.659	10.742	10.851	10.863	10.835	10.823	10.845	11.033	11.031
	2.560	5.301	2.399	2.512	2.451	2.485	2.462	4.590	2.706	3.880
	1.266	2.260	1.194	1.113	1.102	1.156	1.142	2.083	1.576	1.906
	-1.295	-3.042	-1.206	-1.399	-1.349	-1.329	-1.321	-2.508	-1.131	-1.974
	4.677		12.651	12.714	12.584	12.625	12.643		25.909	
BiV	10.204	9.752	11.142	10.424	×	×	10.793	10.240	10.683	10.729
	0.005	2.583	0	0	×	×	2.779	0.044	0	2.974
	1.471	2.219	1.214	1.206	×	×	1.210	2.055	1.030	1.892
	1.467	-0.356	1.283	1.228	×	×	1.255	-0.718	1.072	-1.079
	4.266		13.969	14.757	×	×	14.363		24.601	
BiY	10.833	10.833	10.959	10.964	10.967	10.955	10.962	10.961	11.082	11.089
	2.555	5.292	2.430	2.528	2.496	2.527	2.496	4.584	2.722	3.877
	1.294	2.386	1.200	1.180	1.178	1.229	1.197	2.167	1.620	1.948
	-1.262	-2.906	-1.230	-1.349	-1.318	-1.298	-1.299	-2.418	-1.103	-1.929
	9.767		19.931	20.299	20.131	20.160	20.130		26.480	
BiYb	10.603	10.820	10.763	10.815	10.810	10.791	10.795	10.952	10.987	11.085
	2.790	5.321	1.510	1.866	2.034	1.548	1.740	4.604	2.750	3.887
	1.837	2.150	0.859	1.239	1.340	0.960	1.100	2.010	1.607	1.869
	-0.953	-3.172	-0.652	-0.628	-0.694	-0.588	-0.641	-2.595	-1.143	-2.018
	20.391		33.013	32.563	32.469	32.864	32.727		39.347	
CeDy	10.850	10.859	11.022	10.876	11.025	11.016	10.985	11.041	11.198	11.223
	3.798	5.785	3.701	3.740	3.540	3.681	3.666	5.675	3.312	5.564
	1.571	2.458	1.515	1.480	1.337	1.475	1.452	2.434	1.112	2.409
	-2.228	-3.328	-2.186	-2.260	-2.202	-2.205	-2.214	-3.242	-2.200	-3.155
	0		0	0	0	0	0		0	
CeEr	10.762	10.751	10.956	10.816	10.981	10.964	10.93	10.969	11.167	11.187
	3.781	5.853	3.683	3.719	3.482	3.655	3.635	5.720	3.193	5.587
	1.555	2.440	1.508	1.465	1.291	1.460	1.431	2.422	1.002	2.403
	-2.227	-3.413	-2.175	-2.255	-2.191	-2.195	-2.204	-3.299	-2.191	-3.184
	12.759		24.497	24.325	24.679	24.679	24.545		27.155	
CeEu	10.841	10.955	10.937	10.937	10.937	10.934	10.937	11.105	11.036	11.255
	3.952	5.752	3.882	3.792	3.726	3.852	3.813	5.652	3.556	5.553
	1.664	2.494	1.613	1.517	1.458	1.572	1.540	2.458	1.302	2.421
	-2.289	-3.258	-2.269	-2.275	-2.268	-2.28	-2.273	-3.195	-2.255	-3.132
	13.189		24.766	24.885	24.860	24.844	24.838		27.007	
CeFe	10.011	9.584	10.127	×	10.326	10.368	10.274	10.191	10.827	10.798
	0	1.383	0	×	0.011	0.026	0.013	2.740	0	4.097
	0.433	1.691	0.383	×	0.298	0.377	0.353	1.922	-0.063	2.154
	0.475	0.308	0.414	×	0.288	0.351	0.351	-0.818	-0.053	-1.944
	10.350		15.876	×	21.494	19.990	19.120		0	
CeGa	10.299	9.908	10.364	10.247	10.554	10.553	10.430	10.407	10.945	10.906
	2.292	4.705	2.098	2.654	2.400	2.561	2.429	4.954	1.146	5.204
	0.149	0.990	0.287	0.666	0.595	0.672	0.555	1.455	-0.811	1.920
	-2.144	-3.715	-1.812	-1.989	-1.805	-1.889	-1.874	-3.500	-1.957	-3.284
	7.903		20.381	0	24.413	23.001	16.949		0	
CeGd	10.950	10.962	11.094	10.952	11.099	11.087	11.058	11.110	11.237	11.258
	3.802	5.998	3.710	3.747	3.579	3.687	3.681	5.816	3.412	5.635
	1.575	2.631	1.516	1.489	1.373	1.479	1.465	2.549	1.210	2.467

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	-2.228	-3.367	-2.195	-2.259	-2.206	-2.209	-2.218	-3.268	-2.202	-3.168
	13.541		25.220	24.895	25.331	25.307	25.188		27.605	
CeHo	10.802	10.805	10.987	10.844	10.995	10.981	10.952	11.005	11.180	11.205
	3.792	5.828	3.696	3.730	3.515	3.676	3.655	5.703	3.247	5.578
	1.565	2.422	1.515	1.472	1.316	1.473	1.444	2.410	1.052	2.397
	-2.228	-3.406	-2.181	-2.258	-2.200	-2.203	-2.211	-3.294	-2.195	-3.181
	12.880		24.571	24.347	24.731	24.724	24.593		27.218	
CeIn	10.569	10.58	10.854	10.561	10.821	10.845	10.771	10.855	11.050	11.13
	1.154	3.500	1.791	2.479	2.032	1.979	2.071	4.151	1.745	4.802
	-0.852	0.154	-0.184	0.296	-0.040	-0.073	-0.001	0.898	-0.376	1.641
	-2.006	-3.346	-1.975	-2.183	-2.071	-2.051	-2.070	-3.254	-2.120	-3.161
	0		0	0	0	0	0		0	
CeLa	11.405	11.383	11.401	11.344	11.397	11.399	11.386	11.390	11.404	11.398
	3.444	5.452	3.506	3.627	3.667	3.558	3.590	5.453	3.737	5.453
	1.468	2.329	1.471	1.545	1.569	-3.545	0.260	2.348	1.595	2.366
	-1.976	-3.124	-2.036	-2.082	-2.099	-7.102	-3.330	-3.106	-2.142	-3.087
	28.200		42.394	42.714	43.682	42.819	42.902		4.406	
CeLu	10.628	10.622	10.878	10.77	10.886	10.866	10.85	10.883	11.14	11.144
	3.737	5.913	3.618	3.659	3.412	3.642	3.583	5.760	3.008	5.607
	1.514	2.423	1.477	1.425	1.235	1.457	1.399	2.410	0.836	2.398
	-2.223	-3.491	-2.140	-2.234	-2.178	-2.185	-2.185	-3.350	-2.173	-3.210
	18.309		31.820	32.195	32.266	32.386	32.167		29.320	
CeMn	10.026	9.627	10.157	10.049	10.116	10.477	10.200	10.220	0	10.813
	0	3.033	0	0.001	0.005	0	0.002	3.840	0	4.647
	0.835	1.557	0.682	0.686	0.717	0.703	0.697	1.833	0	2.109
	0.861	-1.477	0.770	0.686	0.713	0.706	0.719	-2.008	0	-2.538
	0		0	0	0	0	0		0	
CePm	11.139	11.155	11.222	11.075	11.224	11.22	11.186	11.238	11.306	11.322
	3.763	5.618	3.698	3.763	3.630	3.682	3.694	5.563	3.545	5.508
	1.548	2.446	1.501	1.510	1.425	-2.080	0.589	2.426	1.345	2.405
	-2.216	-3.172	-2.198	-2.254	-2.205	-5.762	-3.105	-3.138	-2.200	-3.103
	30.489		42.456	32.270	43.820	43.331	40.469		32.864	
CePr	11.3	11.237	11.329	11.18	11.332	11.330	11.293	11.293	11.363	11.349
	3.675	5.588	3.651	3.744	3.630	3.641	3.667	5.543	3.594	5.498
	1.477	2.449	1.459	1.499	1.435	1.448	1.461	2.428	1.404	2.406
	-2.199	-3.139	-2.192	-2.246	-2.196	-2.193	-2.207	-3.115	-2.19	-3.092
	0		0	0	0	0	0		0	
CeSc	10.316	10.288	10.617	10.463	10.675	10.598	10.589	10.660	11.048	11.033
	3.303	6.017	3.601	3.678	3.397	3.748	3.606	5.829	2.806	5.641
	1.691	2.945	1.909	1.781	1.629	1.898	1.805	2.758	0.918	2.572
	-1.612	-3.073	-1.692	-1.897	-1.768	-1.851	-1.802	-3.072	-1.889	-3.070
	10.880		23.162	23.026	23.071	23.426	23.171		25.767	
CeSm	11.093	11.102	11.186	11.038	11.189	11.184	11.150	11.203	11.287	11.304
	3.763	5.636	3.700	3.755	3.615	3.680	3.688	5.575	3.507	5.514
	1.547	2.439	1.503	1.501	1.410	1.475	1.473	2.421	1.306	2.403
	-2.216	-3.198	-2.198	-2.255	-2.206	-2.205	-2.216	-3.155	-2.201	-3.112
	27.374		40.563	38.418	40.889	40.791	40.165		33.625	
CeTb	10.897	10.907	11.051	10.899	11.057	11.047	11.014	11.073	11.209	11.239
	3.808	5.759	3.714	3.756	3.562	3.690	3.681	5.657	3.361	5.555

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.579	2.460	1.520	1.492	1.356	1.481	1.463	2.435	1.159	2.410
	-2.229	-3.300	-2.194	-2.264	-2.207	-2.21	-2.219	-3.223	-2.202	-3.146
	0		0	0	0	0	0		0	
CeTl	10.956	10.926	11.076	10.907	11.101	11.075	11.040	11.086	11.24	11.246
	0.273	1.687	0.785	1.054	0.900	0.845	0.896	2.943	1.047	4.198
	-1.399	-0.906	-1.031	-0.787	-0.921	-5.358	-2.025	0.192	-0.995	1.288
	-1.672	-2.592	-1.815	-1.840	-1.82	-6.203	-2.920	-2.751	-2.042	-2.910
	0		0	0	0	0	0		0	
CeTm	10.708	10.706	10.916	10.778	10.928	10.925	10.887	10.939	11.146	11.172
	3.759	5.872	3.670	3.706	3.464	3.652	3.623	5.732	3.123	5.593
	1.533	2.424	1.504	1.454	1.273	1.461	1.423	2.411	0.937	2.398
	-2.226	-3.449	-2.166	-2.252	-2.191	-2.191	-2.200	-3.322	-2.186	-3.196
	12.525		24.302	24.178	24.49	24.515	24.371		27.015	
CeV	10.089	9.799	10.222	10.193	10.320	10.381	10.279	10.334	10.740	10.870
	0	3.154	0.016	0	0.005	0	0.006	3.921	0	4.687
	1.488	2.383	1.457	1.375	1.371	1.338	1.386	2.383	1.095	2.384
	1.511	-0.763	1.441	1.391	1.367	1.342	1.386	-1.532	1.104	-2.300
	10.312		21.704	21.359	20.731	23.627	21.855		22.845	
CeY	10.876	10.880	11.034	10.883	11.039	11.027	10.996	11.055	11.204	11.230
	3.878	5.863	3.753	3.778	3.591	3.720	3.711	5.726	3.374	5.590
	1.704	2.550	1.592	1.548	1.416	1.543	1.525	2.495	1.189	2.440
	-2.175	-3.314	-2.161	-2.231	-2.175	-2.178	-2.187	-3.232	-2.186	-3.151
	0		0	0	0	0	0		0	0
CeYb	10.865	10.867	11.041	10.825	11.076	11.034	10.994	11.046	11.211	11.226
	4.160	5.892	4.165	4.134	4.002	4.099	4.100	5.746	3.717	5.600
	1.562	2.314	1.595	1.525	1.425	-1.508	0.760	2.338	1.325	2.361
	-2.599	-3.579	-2.570	-2.609	-2.577	-5.606	-3.341	-3.409	-2.392	-3.239
	30.318		42.403	34.375	46.581	43.142	41.625		2.689	
DyEr	10.580	10.569	10.613	×	10.614	10.612	10.613	10.605	10.650	10.641
	3.991	5.963	3.968	×	3.939	3.968	3.959	5.941	3.898	5.918
	0.777	2.464	1.533	×	1.492	1.527	1.518	2.470	1.466	2.476
	1.541	-3.500	-2.435	×	-2.447	-2.442	-2.442	-3.471	-2.433	-3.443
	12.472		23.537	×	23.567	23.549	23.551		22.012	
DyEu	10.749	10.773	10.814	10.704	10.702	10.703	10.731	10.741	10.655	10.709
	3.875	5.862	3.906	3.956	3.971	3.934	3.942	5.873	4.029	5.885
	0.657	2.518	1.509	1.560	1.581	1.535	1.547	2.506	1.627	2.494
	1.485	-3.344	-2.398	-2.396	-2.39	-2.399	-2.396	-3.368	-2.402	-3.391
	10.281		19.344	19.346	19.324	19.344	19.339		22.018	0
DyFe	9.415	9.402	9.789	9.713	9.888	9.845	9.809	9.827	10.282	10.252
	0.015	1.493	0	0	0	0	0	2.961	0	4.428
	0.014	1.715	0.266	0.207	0.220	0.237	0.233	1.971	-0.279	2.226
	0.148	0.222	0.283	0.213	0.221	0.265	0.246	-0.991	-0.250	-2.203
	10.537		20.013	23.422	21.408	22.445	21.822		0	
DyGa	9.840	9.726	10.073	10.086	10.233	10.143	10.134	10.043	10.389	10.36
	1.887	4.815	2.057	2.658	2.539	2.460	2.429	5.175	1.808	5.536
	2.618	1.014	0.139	0.384	0.306	0.310	0.285	1.503	-0.504	1.993
	-0.083	-3.801	-1.919	-2.274	-2.234	-2.151	-2.145	-3.672	-2.312	-3.543
	16.468		27.187	27.127	26.764	27.459	27.134		18.813	
DyGd	10.781	10.780	10.746	10.745	10.746	10.747	10.746	10.745	10.710	10.711

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	3.858	6.109	3.875	3.902	3.913	3.890	3.895	6.038	3.949	5.967
	0.696	2.655	1.492	1.521	1.537	1.507	1.515	2.598	1.565	2.540
	1.480	-3.454	-2.384	-2.381	-2.377	-2.384	-2.382	-3.441	-2.384	-3.427
	12.613		23.689	23.678	23.667	23.684	23.679		26.861	
DyHo	10.630	10.623	10.647	10.646	10.644	10.641	10.645	10.641	10.659	10.659
	3.967	5.939	3.954	3.942	3.942	3.956	3.949	5.924	3.929	5.910
	0.746	2.447	1.531	1.515	1.512	1.528	1.522	2.459	1.502	2.470
	1.538	-3.492	-2.424	-2.428	-2.431	-2.429	-2.428	-3.466	-2.427	-3.440
	12.445		23.485	23.495	23.498	23.489	23.492		22.078	0
DyIn	10.408	10.398	10.497	10.503	10.497	10.500	10.500	10.491	10.587	10.584
	1.565	3.610	2.092	2.171	2.136	2.132	2.133	4.372	2.270	5.134
	3.385	0.178	-0.213	-0.139	-0.189	-0.169	-0.178	0.946	-0.133	1.714
	-0.761	-3.432	-2.305	-2.310	-2.324	-2.300	-2.310	-3.426	-2.403	-3.420
	19.807		27.982	30.306	31.02	29.430	29.685		22.022	
DyLa	11.231	11.201	11.042	11.019	11.026	11.037	11.031	11.026	10.854	10.851
	3.186	5.563	3.332	3.594	3.676	3.491	3.524	5.674	3.912	5.785
	0.835	2.353	1.374	1.562	1.625	1.485	1.512	2.396	1.797	2.439
	1.249	-3.210	-1.958	-2.033	-2.051	-2.007	-2.013	-3.278	-2.116	-3.346
	22.986		36.116	37.123	37.053	36.66	36.738		30.593	
DyLu	10.442	10.439	10.52	10.522	10.523	10.521	10.522	10.518	10.600	10.597
	4.043	6.024	3.996	3.961	3.925	3.981	3.966	5.981	3.816	5.939
	0.890	2.447	1.544	1.485	1.446	1.517	1.498	2.459	1.368	2.471
	1.560	-3.577	-2.453	-2.477	-2.480	-2.464	-2.469	-3.523	-2.448	-3.469
	19.658		32.560	32.719	32.735	32.649	32.666		30.932	
DyMn	9.449	9.445	9.807	9.814	9.897	9.862	9.845	9.855	10.336	10.266
	0	3.144	0	0	0.002	0.001	0.001	4.061	0	4.979
	0.010	1.581	0.701	0.631	0.696	0.685	0.679	1.881	0.267	2.182
	0.551	-1.563	0.774	0.665	0.694	0.684	0.705	-2.180	0.283	-2.797
	0		0	0	0	0	0		0	
DyPm	10.972	10.973	10.875	10.869	10.869	10.875	10.872	10.874	10.772	10.775
	3.646	5.728	3.710	3.803	3.829	3.765	3.777	5.784	3.912	5.840
	0.714	2.471	1.410	1.496	1.532	1.454	1.473	2.474	1.592	2.478
	1.355	-3.258	-2.301	-2.308	-2.298	-2.311	-2.305	-3.310	-2.321	-3.362
	30.204		42.663	42.759	42.396	42.764	42.645		32.764	
DyPr	11.139	11.054	10.986	10.973	10.972	10.983	10.979	10.928	10.827	10.802
	3.428	5.698	3.521	3.684	3.727	3.616	3.637	5.764	3.840	5.830
	0.814	2.474	1.310	1.443	1.494	1.378	1.407	2.476	1.582	2.479
	1.207	-3.225	-2.212	-2.241	-2.233	-2.238	-2.231	-3.288	-2.259	-3.351
	20.292		32.617	33.277	32.762	33.031	32.921		24.319	
DySc	10.107	10.106	10.298	10.301	10.304	10.294	10.300	10.296	10.487	10.486
	3.594	6.128	3.842	3.996	4.003	3.956	3.950	6.050	3.744	5.973
	0.746	2.969	1.916	2.024	2.044	1.992	1.994	2.807	1.671	2.644
	1.771	-3.159	-1.926	-1.973	-1.960	-1.964	-1.956	-3.244	-2.074	-3.329
	11.751		23.021	23.201	23.155	23.131	23.127		26.482	
DySm	10.92	10.919	10.840	10.835	10.836	10.839	10.838	10.838	10.755	10.757
	3.709	5.747	3.760	3.826	3.846	3.801	3.809	5.796	3.926	5.846
	0.713	2.463	1.431	1.497	1.526	1.467	1.481	2.470	1.585	2.476
	1.391	-3.284	-2.329	-2.329	-2.320	-2.334	-2.328	-3.327	-2.341	-3.371

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	25.139		38.168	38.158	38.039	38.177	38.135		32.527	
DyTb	10.726	10.725	10.714	10.713	10.714	10.713	10.714	10.709	10.697	10.693
	3.901	5.869	3.909	3.921	3.925	3.913	3.917	5.878	3.941	5.887
	0.707	2.484	1.509	1.523	1.53	1.514	1.519	2.483	1.544	2.483
	1.506	-3.386	-2.400	-2.399	-2.396	-2.400	-2.399	-3.395	-2.398	-3.405
	0.025		0.007	0	0	0	0.002		0	
DyTl	10.783	10.744	10.745	10.740	10.738	10.730	10.739	10.721	10.706	10.699
	0.380	1.798	0.865	0.846	0.846	0.857	0.854	3.164	1.303	4.530
	2.661	-0.882	-1.104	-1.077	-1.097	-1.083	-1.091	0.240	-0.952	1.361
	-1.427	-2.679	-1.969	-1.922	-1.942	-1.939	-1.943	-2.924	-2.254	-3.169
	0		0	0	0	0	0		0	
DyTm	10.528	10.523	10.576	10.488	10.578	10.574	10.554	10.574	10.628	10.625
	4.007	5.982	3.986	4.062	3.932	3.967	3.987	5.954	3.878	5.925
	0.823	2.448	1.542	1.568	1.475	1.521	1.527	2.459	1.435	2.471
	1.549	-3.535	-2.444	-2.494	-2.458	-2.446	-2.461	-3.495	-2.443	-3.455
	12.421		19.561	19.481	23.546	23.52	21.527		26.835	
DyV	9.679	9.617	9.947	9.969	10.014	9.904	9.959	9.970	10.353	10.323
	0	3.265	0	0.007	0	0	0.002	4.142	0	5.019
	0.073	2.407	1.515	1.397	1.422	1.398	1.433	2.432	1.306	2.457
	1.552	-0.849	1.545	1.390	1.437	1.481	1.464	-1.704	1.314	-2.559
	8.787		19.763	20.419	20.264	20.366	20.203		22.959	
DyY	10.698	10.698	10.692	10.689	10.691	10.691	10.691	10.691	10.685	10.684
	4.021	5.973	3.989	4.001	4.001	3.994	3.997	5.948	3.979	5.922
	0.545	2.574	1.611	1.627	1.633	1.618	1.623	2.543	1.600	2.513
	1.656	-3.400	-2.378	-2.374	-2.368	-2.376	-2.374	-3.405	-2.38	-3.41
	0		0	0	0.039	0	0.010		0.109	
DyYb	10.698	10.685	10.702	10.704	10.700	10.701	10.702	10.682	10.689	10.679
	4.026	6.003	4.407	4.432	4.463	4.415	4.430	5.967	4.263	5.932
	1.532	2.338	1.550	1.556	1.586	1.549	1.561	2.386	1.633	2.434
	-2.494	-3.665	-2.857	-2.877	-2.878	-2.866	-2.870	-3.582	-2.630	-3.498
	4.715		7.041	7.136	7.252	7.072	7.125		6.614	
ErEu	10.721	10.737	10.647	10.640	10.640	10.645	10.643	10.669	10.567	10.601
	3.796	5.885	3.858	3.949	3.979	3.913	3.925	5.918	4.043	5.952
	1.402	2.512	1.450	1.540	1.579	1.500	1.518	2.494	1.627	2.476
	-2.394	-3.373	-2.409	-2.41	-2.400	-2.412	-2.408	-3.425	-2.417	-3.476
	0		0.538	0	0	0	0.135		0.662	
ErFe	9.386	9.366	9.737	9.692	9.815	9.781	9.757	9.755	10.188	10.144
	0.012	1.516	0	0	0	0	0	3.006	0	4.496
	0.149	1.709	0.247	0.189	0.203	0.222	0.216	1.959	-0.328	2.208
	0.137	0.193	0.255	0.198	0.205	0.257	0.229	-1.048	-0.294	-2.288
	0		0	0	0	0	0		0	
ErGa	9.784	9.690	10.007	9.929	10.023	10.066	10.007	9.971	10.293	10.252
	1.859	4.838	2.123	2.867	2.547	2.481	2.505	5.220	1.945	5.603
	-0.157	1.008	0.119	0.469	0.208	0.254	0.263	1.492	-0.450	1.975
	-2.016	-3.830	-2.005	-2.398	-2.34	-2.227	-2.243	-3.729	-2.395	-3.629
	0		0	0	0	0	0		0	
ErGd	10.750	10.744	10.684	10.602	10.683	10.688	10.665	10.674	10.616	10.604
	3.804	6.131	3.849	3.996	3.925	3.877	3.912	6.083	3.981	6.034
	1.414	2.649	1.444	1.561	1.534	1.474	1.504	2.586	1.574	2.522

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	-2.391	-3.482	-2.406	-2.435	-2.392	-2.403	-2.409	-3.497	-2.408	-3.513
	0		0	11.798	0	0	2.95		0	
ErHo	10.600	10.587	10.582	10.501	10.578	10.578	10.56	10.569	10.566	10.551
	3.941	5.961	3.956	4.069	3.976	3.965	3.992	5.969	3.986	5.978
	1.488	2.441	1.493	1.571	1.516	1.502	1.521	2.447	1.523	2.452
	-2.453	-3.521	-2.463	-2.498	-2.46	-2.464	-2.472	-3.523	-2.463	-3.526
	0.132		0.176	0.324	48.883	0.173	12.389		35.376	
ErIn	10.374	10.362	10.436	10.281	10.434	10.427	10.395	10.419	10.489	10.476
	1.604	3.633	2.127	2.405	2.138	2.159	2.208	4.417	2.368	5.202
	-0.765	0.172	-0.235	-0.026	-0.228	-0.195	-0.171	0.934	-0.099	1.696
	-2.369	-3.461	-2.362	-2.431	-2.366	-2.354	-2.379	-3.483	-2.467	-3.506
	0		0	0	0	0	0		0	
ErLa	11.188	11.165	10.979	10.853	10.952	10.972	10.939	10.954	10.769	10.744
	3.107	5.586	3.261	3.633	3.653	3.451	3.500	5.719	3.881	5.852
	1.179	2.347	1.326	1.583	1.624	1.464	1.500	2.384	1.781	2.421
	-1.928	-3.239	-1.935	-2.05	-2.030	-1.987	-2.001	-3.335	-2.100	-3.432
	0		0	0	0	0	0		0	
ErLu	10.412	10.404	10.460	10.415	10.459	10.458	10.448	10.447	10.501	10.490
	4.052	6.046	4.024	4.061	3.973	4.004	4.016	6.026	3.915	6.006
	1.522	2.442	1.521	1.520	1.461	1.493	1.499	2.447	-2.303	2.453
	-2.531	-3.605	-2.504	-2.541	-2.512	-2.510	-2.517	-3.580	-6.223	-3.554
	0		0	0.325	0	0	0.082		0	
ErMn	9.416	9.409	9.748	9.700	9.825	9.804	9.77	9.784	10.221	10.159
	0.004	3.166	0	0	0	0.003	0.001	4.106	0	5.046
	0.555	1.575	0.685	0.628	0.683	0.686	0.671	1.870	0.229	2.164
	0.552	-1.592	0.764	0.672	0.686	0.684	0.702	-2.237	0.257	-2.883
	0		0	0	0	0	0		0	
ErPm	10.938	10.937	10.813	10.706	10.805	10.814	10.785	10.802	10.678	10.668
	3.565	5.751	3.649	3.886	3.826	3.733	3.774	5.829	3.923	5.908
	1.273	2.465	1.519	1.533	1.525	1.418	1.499	2.463	1.591	2.460
	-2.293	-3.287	-2.429	-2.354	-2.301	-2.316	-2.350	-3.367	-2.333	-3.448
	0		0	0	0	0	0		0	
ErPr	11.108	11.019	10.923	10.810	10.907	10.920	10.890	10.857	10.736	10.695
	3.315	5.721	3.440	3.754	3.719	3.577	3.623	5.809	3.832	5.897
	1.099	2.468	1.241	1.476	1.489	1.341	1.387	2.465	1.569	2.461
	-2.216	-3.253	-2.2	-2.278	-2.23	-2.236	-2.236	-3.345	-2.264	-3.437
	0		0	0	0	0	0		0	
ErSc	10.077	10.070	10.236	10.156	10.239	10.231	10.216	10.224	10.598	10.379
	3.656	6.150	3.900	4.121	4.088	4.009	4.030	6.095	4.006	6.041
	1.796	2.963	1.944	2.087	2.116	2.024	2.043	2.795	2.187	2.626
	-1.861	-3.188	-1.956	-2.034	-1.973	-1.986	-1.988	-3.301	2.200	-3.415
	0		0	0	0	0	0		0	
ErSm	10.891	10.884	10.777	10.685	10.772	10.779	10.754	10.767	10.398	10.650
	3.628	5.769	3.709	3.908	3.846	3.774	3.810	5.841	3.869	5.914
	1.310	2.457	1.377	1.532	1.520	1.432	1.466	2.458	2.097	2.458
	-2.318	-3.312	-2.332	-2.376	-2.326	-2.342	-2.344	-3.384	2.149	-3.456
	0		0	0	0	0	0		0	
ErTb	10.702	10.689	10.650	10.556	10.652	10.649	10.627	10.637	10.665	10.585
	3.859	5.892	3.890	4.038	3.942	3.909	3.945	5.923	3.990	5.955



Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.446	2.478	1.463	1.576	1.527	1.484	1.513	2.471	1.561	2.465
	-2.413	-3.414	-2.428	-2.462	-2.415	-2.426	-2.433	-3.452	-2.43	-3.490
	0		0	0.131	0	0	0.033		0	
ErTl	10.740	10.708	10.675	10.565	10.672	10.666	10.645	10.650	10.617	10.592
	0.374	1.820	0.876	0.930	0.832	0.853	0.873	3.209	1.321	4.597
	-1.448	-0.888	-1.125	-1.052	-1.136	-1.116	-1.108	0.228	-0.957	1.343
	-1.822	-2.707	-2.001	-1.981	-1.967	-1.968	-1.980	-2.981	-2.278	-3.255
	0		0	0	0	0	0		0	
ErTm	10.495	10.488	10.466	10.438	10.513	10.513	10.483	10.503	10.534	10.518
	4.007	6.005	4.063	4.086	3.977	3.992	4.030	5.999	3.955	5.992
	1.516	2.442	1.553	1.558	1.481	1.501	1.524	2.447	1.466	2.453
	-2.492	-3.563	-2.510	-2.528	-2.496	-2.492	-2.507	-3.552	-2.490	-3.540
	0		37.487	41.741	0.492	0	19.930		9.697	
ErV	9.641	9.581	9.911	9.805	9.957	9.865	9.885	9.898	10.261	10.216
	0	3.287	0	0	0.012	0	0.003	4.187	0	5.086
	1.542	2.401	1.527	1.425	1.458	1.413	1.456	2.420	1.301	2.439
	1.585	-0.878	1.561	1.477	1.447	1.492	1.495	-1.761	1.310	-2.645
	0		0	0	0	0	0		0	
ErY	10.672	10.662	10.630	10.539	10.625	10.631	10.607	10.619	10.589	10.576
	3.973	5.996	3.981	4.119	4.029	3.996	4.032	5.993	4.031	5.989
	-2.136	2.568	1.576	1.684	1.641	1.596	1.625	2.531	1.623	2.495
	-6.109	-3.428	-2.406	-2.435	-2.388	-2.401	-2.408	-3.462	-2.408	-3.495
	0		0	0.128	0	0	0.032		0	
ErYb	10.664	10.649	10.631	10.508	10.632	10.631	10.601	10.610	10.589	10.572
	3.990	6.025	4.420	4.634	4.520	4.445	4.505	6.012	4.315	5.999
	-1.378	2.332	1.510	1.648	1.582	1.524	1.566	2.374	1.639	2.416
	-5.368	-3.694	-2.911	-2.986	-2.939	-2.922	-2.940	-3.638	-2.676	-3.583
	0.040		0.047	0.058	0.057	0.049	0.053		0.045	
EuFe	9.442	9.434	9.812	9.809	9.908	9.833	9.841	9.891	10.267	10.348
	0	1.482	0	0.005	0	0	0.002	2.938	0	4.395
	0.127	1.727	-3.842	0.231	0.256	0.263	-0.773	1.995	-0.112	2.263
	0.137	0.245	-3.808	0.227	0.261	0.277	-0.761	-0.944	-0.088	-2.132
	0		0	0	0	0	0		0	
EuGa	9.817	9.758	10.113	10.087	10.147	10.059	10.102	10.107	10.41	10.456
	2.074	4.804	2.091	2.745	2.622	2.411	2.468	5.153	1.638	5.502
	0.069	1.026	0.249	0.547	0.497	0.434	0.432	1.528	-0.591	2.029
	-2.005	-3.778	-1.843	-2.199	-2.125	-1.977	-2.036	-3.626	-2.229	-3.473
	0		0	0	0	0	0		0	
EuGd	10.753	10.812	10.806	10.774	10.773	10.772	10.782	10.810	10.793	10.808
	3.977	6.097	3.914	3.941	3.935	3.945	3.934	6.015	3.911	5.933
	1.598	2.668	1.560	1.566	1.558	1.571	1.564	2.622	1.540	2.576
	-2.379	-3.430	-2.355	-2.376	-2.377	-2.374	-2.371	-3.394	-2.371	-3.357
	24.452		38.507	47.578	47.610	47.443	45.285		0.065	
EuHo	10.607	10.655	10.700	10.666	10.671	10.671	10.677	10.705	10.735	10.755
	4.051	5.927	3.959	3.963	3.925	3.973	3.955	5.902	3.839	5.876
	1.638	2.459	1.587	1.556	1.518	1.577	1.560	2.483	1.445	2.507
	-2.414	-3.469	-2.373	-2.408	-2.407	-2.395	-2.396	-3.420	-2.395	-3.370
	0.341		42.689	0.449	0.462	0.449	11.012		0.340	
EuIn	10.330	10.430	10.493	10.451	10.449	10.439	10.458	10.555	10.570	10.680

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.639	3.599	2.193	2.396	2.330	2.348	2.317	4.350	2.255	5.100
	-0.657	0.191	-0.086	0.080	-0.001	-5.523	-1.383	0.971	-0.128	1.751
	-2.296	-3.409	-2.278	-2.316	-2.331	-7.871	-3.699	-3.380	-2.382	-3.350
	0		0	0	0	0	0		0	
EuLa	11.209	11.233	11.120	11.084	11.085	11.092	11.096	11.090	10.977	10.948
	3.315	5.552	3.432	3.659	3.740	3.570	3.601	5.651	3.928	5.751
	1.358	2.365	1.430	1.583	1.640	1.517	1.543	2.420	1.781	2.475
	-1.957	-3.187	-2.003	-2.076	-2.100	-2.053	-2.058	-3.232	-2.148	-3.276
	0		0	0	0	0	0		0	
EuLu	10.461	10.472	10.604	10.543	10.543	10.538	10.557	10.583	10.706	10.694
	4.026	6.013	3.929	3.944	3.878	3.986	3.935	5.959	3.643	5.905
	1.601	2.460	1.567	1.519	1.449	1.576	1.528	2.483	1.259	2.507
	-2.426	-3.554	-2.363	-2.426	-2.429	-2.41	-2.407	-3.476	-2.383	-3.398
	0		0	0	0	0	0		0	
EuMn	9.536	9.477	9.878	9.854	9.942	9.858	9.883	9.920	0	10.363
	0	3.133	0	0	0.012	0	0.003	4.039	0	4.945
	0.686	1.593	0.705	0.629	0.705	0.693	0.683	1.906	0	2.218
	0.693	-1.540	0.790	0.669	0.694	0.710	0.716	-2.134	0	-2.727
	0		0	0	0	0	0		0	
EuPm	10.931	11.005	10.927	10.892	10.994	10.897	10.928	10.938	10.854	10.872
	3.818	5.717	3.812	3.880	3.890	3.856	3.860	5.762	3.939	5.806
	1.499	2.483	1.501	1.554	1.569	1.531	1.539	2.499	1.607	2.515
	-2.320	-3.235	-2.312	-2.326	-2.321	-2.325	-2.321	-3.264	-2.333	-3.292
	0.007		0	0.003	0.003	0.004	0.003		0	
EuPr	11.081	11.087	11.034	10.993	10.329	10.996	10.838	10.993	10.918	10.899
	3.635	5.687	3.654	3.773	3.810	3.736	3.744	5.742	3.878	5.796
	1.368	2.486	1.412	1.503	1.542	1.465	1.481	2.501	1.600	2.516
	-2.267	-3.202	-2.242	-2.271	-2.269	-2.271	-2.264	-3.241	-2.278	-3.281
	0		0	0	0	0	0		0	
EuSc	10.116	10.138	10.348	10.320	10.861	10.307	10.459	10.360	10.528	10.583
	3.529	6.116	3.784	3.931	3.868	3.929	3.878	6.028	3.520	5.939
	1.748	2.981	1.890	1.960	1.926	1.962	1.935	2.831	1.445	2.681
	-1.782	-3.136	-1.895	-1.972	-1.942	-1.967	-1.944	-3.198	-2.075	-3.259
	0		0	0	0	0	0		0	
EuSm	10.877	10.952	10.894	10.861	10.726	10.862	10.836	10.903	10.839	10.854
	3.868	5.735	3.845	3.894	3.903	3.886	3.882	5.774	3.926	5.812
	1.529	2.475	1.518	1.554	1.564	1.543	1.545	2.494	1.584	2.512
	-2.34	-3.261	-2.327	-2.341	-2.339	-2.343	-2.338	-3.281	-2.343	-3.301
	0.067		0.013	0.034	0.031	0.036	0.028		0.011	
EuTb	10.694	10.757	10.728	10.728	10.737	10.725	10.73	10.773	10.760	10.789
	4.013	5.858	3.964	3.964	3.947	3.977	3.963	5.856	3.904	5.853
	1.619	2.496	1.572	1.572	1.554	1.588	1.572	2.507	1.519	2.519
	-2.394	-3.363	-2.393	-2.392	-2.394	-2.389	-2.392	-3.349	-2.385	-3.335
	0.125		0.045	0.045	0.047	0.031	0.042		0.009	
EuTl	10.709	10.776	10.776	10.743	10.597	10.731	10.712	10.786	10.768	10.796
	0.419	1.786	0.905	0.965	0.968	0.962	0.950	3.141	1.361	4.496
	-1.390	-0.870	-1.038	-0.950	-0.965	-0.969	-0.981	0.265	-0.884	1.398
	-1.809	-2.655	-1.942	-1.915	-1.932	-1.930	-1.930	-2.877	-2.244	-3.099

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0		0	0	0	0	0		0	
EuTm	10.519	10.556	10.636	10.609	10.597	10.604	10.612	10.639	10.699	10.722
	4.043	5.971	3.958	3.935	3.902	3.972	3.942	5.931	3.750	5.891
	1.622	2.460	1.586	1.523	1.480	1.571	1.540	2.484	1.353	2.507
	-2.421	-3.512	-2.373	-2.413	-2.422	-2.401	-2.403	-3.448	-2.397	-3.384
	32.125		29.800	41.823	38.965	38.257	37.211		25.572	
EuV	9.722	9.649	9.955	9.722	10.021	9.904	9.901	10.034	10.334	10.420
	0	3.254	0	0.278	0	0	0.070	4.119	0	4.985
	1.552	2.419	-0.029	0.936	1.428	1.411	0.937	2.456	1.331	2.493
	1.562	-0.826	0.072	0.658	1.463	1.43	0.906	-1.658	1.332	-2.489
	0		0	0	0	0	0		0	
EuY	10.666	10.730	10.745	10.713	10.712	10.707	10.72	10.755	10.754	10.78
	4.127	5.962	4.011	4.014	3.999	4.032	4.014	5.925	3.924	5.888
	1.768	2.586	1.671	1.655	1.641	1.674	1.661	2.568	1.561	2.549
	-2.359	-3.376	-2.341	-2.359	-2.359	-2.359	-2.355	-3.358	-2.364	-3.339
	0.046		0.058	0.037	0.047	0.008	0.038		0.023	
EuYb	10.626	10.717	10.733	10.686	10.690	10.688	10.700	10.746	10.737	10.776
	4.355	5.992	4.440	4.439	4.445	4.451	4.444	5.945	4.237	5.898
	1.661	2.350	1.642	1.617	1.628	1.637	1.631	2.410	1.638	2.470
	-2.695	-3.642	-2.799	-2.822	-2.818	-2.815	-2.814	-3.535	-2.599	-3.428
	0.011		0.037	0.032	0.046	0.026	0.035		0.045	
FeGa	9.318	9.301	9.203	9.204	9.219	9.203	9.208	9.193	9.108	9.085
	0	3.348	0.010	0.005	0	0	0.004	2.240	0	1.133
	-0.487	0.758	0.076	0.120	0.153	0.088	0.110	0.992	0.266	1.226
	-0.420	-2.590	0.066	0.116	0.177	0.088	0.112	-1.249	0.273	0.093
	0		0	0	0	0	0		0	
FeGd	10.387	10.355	9.915	9.837	9.716	9.931	9.850	9.896	9.449	9.437
	0	4.641	0	0	0	0	0	3.103	0.008	1.564
	-0.224	2.400	0.213	0.228	0.249	0.242	0.233	2.086	0.137	1.773
	-0.200	-2.242	0.286	0.237	0.271	0.258	0.263	-1.017	0.129	0.209
	9.597		21.468	23.692	23.630	23.020	22.953		22.890	
FeHo	10.239	10.198	9.813	9.697	9.655	9.845	9.753	9.791	9.400	9.384
	0	4.471	0	0	0	0	0	2.989	0.017	1.508
	-0.303	2.191	0.205	0.189	0.230	0.212	0.209	1.947	0.152	1.703
	-0.200	-2.281	0.268	0.198	0.262	0.212	0.235	-1.043	0.136	0.196
	10.307		22.349	24.038	23.779	23.417	23.395		23.834	
FeIn	9.982	9.973	9.657	9.533	9.669	9.705	9.641	9.641	0	9.309
	0	2.143	0	0	0	0	0	1.437	0	0.732
	-0.271	-0.078	0.123	0.146	0.171	0.188	0.157	0.435	0	0.947
	-0.211	-2.221	0.145	0.167	0.196	0.197	0.177	-1.003	0	0.216
	0		0	0	0	0	0		0	
FeLa	10.804	10.776	10.199	10.006	10.066	10.014	10.072	10.176	9.986	9.577
	0	4.096	0	0	0.020	0.031	0.013	2.739	0	1.383
	-0.009	2.098	0.199	0.274	0.379	0.285	0.285	1.885	0.419	1.672
	0.052	-1.998	0.279	0.288	0.359	0.254	0.295	-0.855	0.457	0.290
	0		0	0	0	0	0		0	
FeLu	10.054	10.015	9.690	9.665	9.613	9.716	9.671	9.669	9.340	9.323
	0	4.556	0	0	0	0	0	3.046	0.018	1.536
	-0.398	2.192	0.185	0.167	0.205	0.175	0.183	1.948	0.163	1.703

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	-0.357	-2.365	0.238	0.202	0.237	0.179	0.214	-1.099	0.145	0.168
	13.513		23.382	25.940	25.108	25.139	24.892		17.108	
FeMn	9.020	9.020	9.011	9.009	9.015	9.012	9.012	9.006	8.987	8.992
	0	1.676	0	0	0	0	0	1.126	0	0.576
	0.310	1.325	0.205	0.198	0.201	0.198	0.201	1.370	0.101	1.415
	0.310	-0.352	0.247	0.228	0.246	0.220	0.236	0.244	0.162	0.839
	0.744		0.302	0.015	0	0.178	0.124		0	
FePm	10.567	10.548	10.044	9.99	9.815	10.085	9.984	10.024	9.513	9.501
	0	4.261	0	0	0	0	0	2.849	0	1.438
	-0.146	2.215	0.225	0.263	0.272	0.333	0.274	1.963	0.118	1.711
	-0.127	-2.046	0.304	0.284	0.310	0.347	0.312	-0.887	0.122	0.274
	0		0	0	0	0	0		0	0
FePr	10.710	10.63	10.153	9.960	9.969	10.202	10.071	10.079	9.928	9.528
	0	4.231	0	0	0.028	0	0.007	2.829	0	1.428
	-0.076	2.218	0.242	0.285	0.367	0.326	0.305	1.965	0.429	1.712
	-0.065	-2.013	0.313	0.293	0.339	0.341	0.322	-0.865	0.462	0.285
	0		0	0	0	0	0		0	
FeSc	9.698	9.681	9.452	9.434	9.443	9.460	9.448	9.446	9.226	9.212
	0	4.66	0	0	0	0	0	3.115	0.001	1.571
	-0.041	2.713	0.242	0.226	0.259	0.234	0.241	2.295	0.142	1.877
	0.001	-1.947	0.271	0.255	0.286	0.234	0.262	-0.821	0.142	0.307
	13.567		26.107	26.681	26.15	26.558	26.374		26.305	
FeSm	10.513	10.495	10.007	9.756	9.787	10.013	9.891	9.989	9.492	9.483
	0	4.279	0	0	0	0	0	2.862	-0.004	1.444
	-0.166	2.207	0.221	0.228	0.267	0.339	0.264	1.958	0.120	1.709
	-0.146	-2.072	0.297	0.234	0.302	0.351	0.296	-0.904	0.124	0.265
	0		0	0	0	0	0		0	
FeTb	10.328	10.300	9.879	9.749	9.692	9.899	9.805	9.859	9.433	9.418
	0	4.402	0	0	0	0	0	2.943	0.012	1.485
	-0.256	2.228	0.212	0.203	0.243	0.227	0.222	1.972	0.142	1.715
	-0.229	-2.174	0.280	0.205	0.270	0.232	0.247	-0.972	0.131	0.231
	0		0	0	0	0	0		0	
FeTl	10.307	10.319	9.919	10.076	11.130	10.121	10.312	9.872	9.452	9.425
	0	0.330	0	0	0.004	0.010	0.004	0.229	-0.034	0.127
	0.016	-1.137	0.193	0.243	0.577	0.383	0.349	-0.272	0.163	0.594
	-0.052	-1.467	0.198	0.243	0.574	0.373	0.347	-0.500	0.196	0.467
	0		0	0	0.033	0	0.009		0	
FeTm	10.13	10.099	9.693	9.574	9.622	9.775	9.666	9.725	9.369	9.351
	0	4.515	0	0	0	0	0	3.019	0.022	1.522
	-0.352	2.192	0.206	0.184	0.218	0.192	0.200	1.948	0.162	1.703
	-0.316	-2.323	0.264	0.195	3.000	0.196	0.914	-1.071	0.140	0.182
	10.871		23.075	24.691	24.082	23.936	23.946		24.378	0
FeV	9.213	9.192	9.132	9.138	9.138	9.158	9.142	9.120	9.050	9.049
	0	1.797	0	0	0.018	0	0.005	1.207	0	0.616
	1.046	2.151	0.662	0.626	0.673	0.660	0.656	1.920	0.290	1.690
	1.118	0.363	0.668	0.654	0.655	0.664	0.661	0.720	0.426	1.077
	10.194		17.585	17.484	17.415	17.831	17.579		16.710	
FeY	10.294	10.273	9.858	9.749	9.695	9.895	9.800	9.841	9.423	9.409
	0	4.506	0	0	0	0.002	0.001	3.013	0.012	1.519

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	-0.230	2.318	0.214	0.205	0.241	0.234	0.224	2.032	0.147	1.745
	-0.201	-2.188	0.276	0.216	0.273	0.233	0.250	-0.981	0.136	0.227
	0		0	0	0	0	0		0	
FeYb	10.03	10.260	9.653	9.549	9.521	9.774	9.625	9.832	9.302	9.405
	0	4.535	0	0	0	0.001	0.001	3.032	0.003	1.529
	-1.525	2.083	-0.135	-0.028	-0.028	-0.128	-0.080	1.875	0.087	1.667
	-1.469	-2.453	-0.122	-0.015	-0.011	-0.129	-0.070	-1.158	0.084	0.138
	8.560		17.411	16.493	16.751	16.879	16.884		15.148	
GaGd	10.498	10.463	10.198	10.010	10.169	10.27	10.162	10.112	9.920	9.761
	1.662	5.748	2.229	2.529	2.372	2.543	2.419	5.317	1.993	4.886
	-0.564	2.166	0.141	0.402	0.409	0.438	0.348	1.619	-0.298	1.072
	-2.226	-3.583	-2.088	-2.127	-1.963	-2.105	-2.071	-3.699	-2.291	-3.815
	11.762		24.219	24.577	24.785	24.779	24.590		23.781	
GaHo	10.339	10.306	10.088	9.961	9.898	10.034	9.996	10.007	9.808	9.708
	1.879	5.578	2.311	2.677	2.472	2.522	2.496	5.204	1.865	4.829
	-0.475	1.957	0.153	0.365	0.282	0.226	0.257	1.480	-0.827	1.002
	-2.353	-3.621	-2.159	-2.312	-2.190	-2.296	-2.240	-3.725	-2.692	-3.828
	12.421		24.606	24.841	24.901	24.574	24.730		26.267	
GaIn	10.066	10.081	9.855	9.854	9.838	9.860	9.852	9.857	9.632	9.633
	1.068	3.250	1.262	1.284	1.287	1.278	1.278	3.652	1.614	4.053
	-1.300	-0.312	-1.114	-1.108	-1.097	-1.101	-1.105	-0.033	-0.896	0.246
	-2.368	-3.562	-2.376	-2.391	-2.384	-2.378	-2.383	-3.685	-2.509	-3.808
	0		0	0	0	0	0		0	
GaLa	10.935	10.884	10.537	10.246	10.598	10.514	10.474	10.392	10.288	9.901
	1.299	5.203	1.854	2.727	2.919	2.452	2.488	4.953	2.462	4.704
	-0.428	1.864	0.265	1.065	1.196	0.983	0.878	1.418	0.480	0.971
	-1.726	-3.339	-1.589	-1.663	-1.723	-1.470	-1.612	-3.536	-1.983	-3.733
	0		0	0	0	0	0		0	
GaLu	10.146	10.123	9.915	9.791	9.839	9.908	9.864	9.885	9.685	9.647
	2.153	5.664	2.287	2.930	2.583	2.648	2.612	5.261	1.910	4.858
	-0.360	1.958	-0.152	0.416	0.207	0.174	0.162	1.480	-0.28	1.003
	-2.513	-3.706	-2.438	-2.514	-2.377	-2.474	-2.451	-3.781	-2.19	-3.856
	19.010		30.760	32.408	31.458	31.443	31.517		25.427	
GaMn	9.115	9.128	9.248	9.215	9.236	7.997	8.924	9.222	9.338	9.316
	3.854	2.784	0	0.01	0	0	0.003	3.341	0	3.898
	0.607	1.092	0.674	0.643	0.609	0.648	0.644	0.903	-13.920	0.714
	0.644	-1.692	0.700	0.632	0.610	0.658	0.650	-2.438	-13.871	-3.184
	0		0	0	0	0	0		0	
GaPm	10.687	10.656	10.333	10.100	10.238	10.579	10.313	10.24	10.120	9.825
	1.421	5.368	2.108	2.422	2.439	2.620	2.398	5.064	2.178	4.759
	-0.670	1.981	0.105	0.435	0.483	0.530	0.389	1.496	-0.045	1.010
	-2.090	-3.387	-2.004	-1.987	-1.957	-2.090	-2.010	-3.568	-2.223	-3.749
	0		0	0	0	0	0		0	
GaPr	10.850	10.738	10.453	10.293	10.315	10.459	10.380	10.295	10.238	9.852
	1.237	5.338	1.900	2.531	2.419	2.474	2.331	5.044	2.277	4.749
	-0.762	1.984	0.038	0.566	0.510	0.684	0.450	1.498	0.106	1.011
	-1.999	-3.354	-1.863	-1.966	-1.909	-1.791	-1.883	-3.546	-2.171	-3.738
	0		0	0	0	0	0		0	
GaSc	9.798	9.789	9.670	9.663	9.660	9.672	9.667	9.662	9.554	9.536

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	2.639	5.767	2.812	3.254	3.146	3.136	3.087	5.330	2.627	4.892
	0.739	2.480	0.886	1.36	1.274	1.224	1.186	1.828	0.492	1.176
	-1.901	-3.288	-1.926	-1.894	-1.873	-1.913	-1.902	-3.502	-2.136	-3.716
	15.172		27.186	27.193	27.044	27.254	27.169		27.529	
GaSm	10.640	10.603	10.292	9.980	10.227	10.501	10.250	10.205	10.067	9.807
	1.481	5.386	2.153	2.682	2.378	2.688	2.476	5.076	2.139	4.765
	-0.641	1.974	0.113	0.563	0.457	0.567	0.425	1.491	-0.107	1.008
	-2.122	-3.413	-2.040	-2.120	-1.921	-2.120	-2.051	-3.586	-2.245	-3.758
	11.923		0	0	20.505	24.033	11.135		0	
GaTb	10.438	10.408	10.161	9.988	9.941	10.216	10.077	10.075	9.876	9.742
	1.741	5.509	2.256	2.615	2.441	2.561	2.469	5.158	1.902	4.806
	-0.531	1.994	0.147	0.394	0.339	0.406	0.322	1.505	-0.049	1.015
	-2.271	-3.515	-2.109	-2.221	-2.102	-2.156	-2.147	-3.654	-1.950	-3.792
	0		0	0	0	0	0		0	
GaTl	10.41	10.427	10.083	10.074	10.037	10.121	10.079	10.088	9.798	9.749
	0	1.437	0.034	0.007	0.010	0.018	0.018	2.443	0.711	3.449
	-1.737	-1.371	-1.758	-1.838	-1.789	-1.802	-1.797	-0.739	-1.533	-0.108
	-1.707	-2.808	-1.791	-1.844	-1.798	-1.819	-1.813	-3.182	-2.243	-3.556
	0		0	0	0	0	0		0	
GaTm	10.235	10.207	10.015	9.807	9.859	9.960	9.911	9.941	9.752	9.675
	2.018	5.622	2.379	2.927	2.506	2.579	2.598	5.233	1.867	4.844
	-0.423	1.959	0.139	0.479	0.231	0.195	0.261	1.481	-0.189	1.003
	-2.440	-3.664	-2.241	-2.449	-2.276	-2.384	-2.338	-3.753	-2.056	-3.842
	12.973		25.454	25.504	25.260	25.140	25.339		26.424	
GaV	9.353	9.300	9.373	9.345	9.485	9.389	9.398	9.336	9.431	9.373
	0	2.905	0	0.015	0	0	0.004	3.421	0	3.938
	1.551	1.918	1.479	1.436	1.309	1.343	1.392	1.453	1.111	0.989
	1.603	-0.979	1.564	1.421	1.322	1.393	1.425	-1.963	1.175	-2.947
	13.516		26.127	26.882	26.899	26.835	26.686		26.850	
GaY	10.399	10.381	10.138	9.890	9.938	10.168	10.034	10.057	9.850	9.733
	1.878	5.613	2.328	2.952	2.500	2.597	2.595	5.227	1.925	4.841
	-0.379	2.085	0.270	0.678	0.419	0.444	0.453	1.565	0.022	1.045
	-2.256	-3.529	-2.058	-2.274	-2.081	-2.154	-2.142	-3.663	-1.903	-3.797
	0		0	0	0	0	0		0	
GaYb	10.302	10.368	10.056	10.035	10.023	10.257	10.093	10.048	9.836	9.729
	3.134	5.643	0.065	0.022	0	0	0.022	5.247	2.302	4.851
	-0.163	1.849	0.884	0.982	1.120	1.549	1.134	1.408	-0.333	0.966
	-3.296	-3.794	0.819	0.960	1.043	2.061	1.221	-3.840	-2.634	-3.885
	3.505		18.450	24.365	25.149	25.723	23.422		2.434	
GdHo	10.658	10.658	10.715	10.715	10.712	10.711	10.714	10.710	10.768	10.762
	3.968	6.010	3.931	3.909	3.883	3.924	3.912	6.066	3.828	6.123
	1.572	2.504	1.556	1.517	1.489	1.539	1.526	2.574	1.445	2.644
	-2.397	-3.506	-2.376	-2.392	-2.394	-2.386	-2.387	-3.493	-2.383	-3.480
	31.820		44.113	46.263	46.706	45.255	45.584		36.181	
GdIn	10.446	10.433	10.575	10.583	10.571	10.569	10.575	10.560	10.690	10.687
	1.486	3.681	2.047	2.157	2.121	2.111	2.109	4.514	2.159	5.347
	-0.769	0.236	-0.206	-0.106	-0.158	-0.138	-0.152	1.062	-0.180	1.888
	-2.254	-3.446	-2.252	-2.263	-2.279	-2.249	-2.261	-3.453	-2.338	-3.460

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0		0	0	0	0	0		0	
GdLa	11.256	11.235	11.116	10.996	11.097	11.109	11.080	11.095	10.957	10.955
	3.281	5.634	3.410	3.684	3.699	3.533	3.582	5.816	3.910	5.998
	1.330	2.411	1.421	1.6	1.629	1.505	1.539	2.512	1.784	2.613
	-1.951	-3.223	-1.990	-2.084	-2.070	-2.029	-2.044	-3.304	-2.127	-3.386
	0		0	0	0	0	0		0	
GdLu	10.475	10.474	10.591	10.596	10.593	10.589	10.593	10.587	10.706	10.701
	3.998	6.095	3.954	3.897	3.844	3.927	3.906	6.123	3.688	6.151
	1.566	2.505	1.563	1.479	1.422	1.525	1.498	2.575	1.293	2.644
	-2.433	-3.590	-2.391	-2.418	-2.423	-2.403	-2.409	-3.549	-2.395	-3.508
	0		0	0	0	0	0		0	
GdMn	9.500	9.479	9.875	9.946	9.987	9.951	9.940	9.924	10.401	10.369
	0.004	3.215	0	0	0	0	0	4.203	0	5.191
	0.592	1.639	0.710	0.664	0.627	0.707	0.677	1.997	-6.794	2.355
	0.589	-1.576	0.787	0.683	0.631	0.726	0.707	-2.207	-6.791	-2.837
	0		0	0	0	0	0		0	
GdPm	11.01	11.007	10.945	10.941	10.944	10.944	10.944	10.943	10.883	10.879
	3.719	5.799	3.763	3.812	3.823	3.789	3.797	5.926	3.880	6.053
	1.432	2.528	1.464	1.514	1.533	1.489	1.500	2.590	1.577	2.652
	-2.288	-3.271	-2.300	-2.298	-2.29	-2.301	-2.298	-3.336	-2.304	-3.402
	0		0	0	0	0	0		0	
GdPr	11.169	11.089	11.056	11.047	11.047	11.053	11.051	10.997	10.936	10.906
	3.519	5.769	3.592	3.700	3.731	3.657	3.670	5.906	3.825	6.043
	1.294	2.531	1.372	1.461	1.499	1.418	1.438	2.592	1.574	2.653
	-2.226	-3.238	-2.220	-2.239	-2.232	-2.240	-2.233	-3.314	-2.252	-3.391
	0		0	0	0	0	0		0	
GdSc	10.149	10.140	10.367	10.371	10.377	10.361	10.369	10.365	10.598	10.590
	3.530	6.199	3.777	3.917	3.884	3.895	3.869	6.192	3.564	6.186
	1.752	3.027	1.889	1.971	1.960	1.958	1.945	2.922	1.527	2.818
	-1.778	-3.172	-1.889	-1.946	-1.925	-1.937	-1.925	-3.270	-2.037	-3.369
	0		0	0	0	0	0		0	
GdSm	10.956	10.954	10.911	10.908	10.909	10.912	10.91	10.907	10.865	10.861
	3.765	5.818	3.792	3.824	3.834	3.810	3.815	5.938	3.882	6.059
	1.458	2.521	1.478	1.511	1.526	1.495	1.503	2.585	1.563	2.649
	-2.307	-3.297	-2.315	-2.313	-2.309	-2.316	-2.314	-3.354	-2.32	-3.410
	0		0	0	0	0	0		0	
GdTb	10.764	10.760	10.783	10.784	10.781	10.778	10.782	10.778	10.801	10.796
	3.920	5.940	3.903	3.894	3.891	3.904	3.898	6.020	3.871	6.100
	1.550	2.542	1.540	1.526	1.521	1.537	1.531	2.599	1.507	2.656
	-2.371	-3.399	-2.363	-2.369	-2.371	-2.367	-2.368	-3.422	-2.365	-3.444
	0		0	0	0	0	0		0.004	
GdTl	10.815	10.778	10.815	10.817	10.811	10.804	10.812	10.790	10.824	10.802
	0.372	1.869	0.848	0.861	0.861	0.860	0.858	3.306	1.250	4.742
	-1.416	-0.824	-1.090	-1.035	-1.053	-1.051	-1.058	0.356	-0.968	1.535
	-1.788	-2.692	-1.937	-1.896	-1.913	-1.910	-1.914	-2.950	-2.217	-3.208
	0		0	0	0	0	0		0	
GdTm	10.559	10.558	10.647	10.569	10.647	10.645	10.627	10.643	10.734	10.729
	3.992	6.053	3.947	3.990	3.863	3.922	3.931	6.095	3.759	6.137
	1.572	2.506	1.558	1.548	1.452	1.526	1.521	2.575	1.366	2.644

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	-2.421	-3.548	-2.389	-2.442	-2.412	-2.396	-2.410	-3.521	-2.394	-3.494
	23.834		0.324	0.315	36.771	34.343	17.938		27.581	
GdV	9.750	9.651	9.998	9.937	10.086	9.950	9.993	10.039	10.447	10.427
	0.005	3.336	0	0.011	0	0	0.003	4.284	0	5.232
	1.555	2.465	1.500	1.407	1.411	1.383	1.426	2.548	1.314	2.630
	1.551	-0.863	1.554	1.396	1.440	1.439	1.458	-1.731	1.318	-2.599
	0		0	0	0	0	0		0	
GdY	10.735	10.733	10.762	10.763	10.760	10.761	10.762	10.760	10.792	10.787
	4.033	6.044	3.974	3.961	3.951	3.966	3.963	6.089	3.899	6.134
	1.696	2.632	1.637	1.620	1.612	1.627	1.624	2.659	1.554	2.686
	-2.337	-3.413	-2.337	-2.342	-2.339	-2.340	-2.340	-3.431	-2.345	-3.449
	0		0	0	0.002	0	0.001		0.017	
GdYb	10.739	10.719	10.781	10.775	10.774	10.778	10.777	10.751	10.798	10.783
	4.039	6.074	4.376	4.375	4.390	4.369	4.378	6.109	4.193	6.144
	1.559	2.396	1.580	1.558	1.579	1.562	1.57	2.502	1.613	2.608
	-2.481	-3.678	-2.796	-2.817	-2.811	-2.807	-2.808	-3.608	-2.581	-3.537
	0.019		0.034	0.043	0.053	0.037	0.042		0.050	
HoIn	10.392	10.380	10.466	10.476	10.465	10.468	10.469	10.455	10.533	10.530
	1.587	3.625	2.111	2.161	2.139	2.139	2.138	4.401	2.322	5.177
	-0.763	0.167	-0.223	-0.166	-0.206	-0.186	-0.196	0.923	-0.114	1.679
	-2.349	-3.459	-2.334	-2.327	-2.345	-2.324	-2.333	-3.478	-2.436	-3.498
	0		0	0	0	0	0		0	
HoLa	11.209	11.183	11.009	10.884	10.987	11.004	10.971	10.990	10.806	10.798
	3.155	5.577	3.294	3.646	3.670	3.470	3.520	5.702	3.907	5.828
	1.221	2.342	1.351	1.589	1.627	1.475	1.511	2.373	1.798	2.404
	-1.935	-3.236	-1.944	-2.057	-2.043	-1.996	-2.010	-3.330	-2.11	-3.424
	0		0	0	0	0	0		0	
HoLu	10.423	10.422	10.489	10.488	10.490	10.488	10.489	10.483	10.550	10.544
	4.053	6.038	4.011	3.981	3.953	3.999	3.986	6.010	3.872	5.981
	1.543	2.436	1.531	1.480	1.448	1.505	1.491	2.435	1.398	2.435
	-2.510	-3.603	-2.481	-2.502	-2.506	-2.495	-2.496	-3.575	-2.475	-3.547
	0		0	0	0	0	0		0	
HoMn	9.434	9.427	9.779	9.712	9.859	9.829	9.795	9.820	10.245	10.213
	0.003	3.158	0	0	0.005	0.002	0.002	4.090	0	5.021
	0.552	1.569	0.692	0.624	0.695	0.685	0.674	1.858	-6.675	2.146
	0.550	-1.589	0.768	0.674	0.690	0.683	0.704	-2.232	-6.675	-2.875
	0		0	0	0	0	0		0	
HoPm	10.959	10.955	10.845	10.752	10.835	10.841	10.819	10.838	10.726	10.722
	3.608	5.743	3.681	3.884	3.830	3.751	3.787	5.813	3.921	5.883
	1.317	2.459	1.382	1.538	1.529	1.437	1.472	2.451	1.595	2.443
	-2.292	-3.284	-2.300	-2.347	-2.301	-2.314	-2.316	-3.362	-2.327	-3.440
	0		0	0	0	0	0		0	
HoPr	11.12	11.037	10.953	10.841	10.939	10.949	10.921	10.893	10.777	10.749
	3.378	5.712	3.482	3.762	3.723	3.599	3.642	5.793	3.846	5.873
	1.157	2.462	1.276	1.484	1.492	1.361	1.404	2.453	1.584	2.444
	-2.221	-3.251	-2.206	-2.279	-2.232	-2.239	-2.239	-3.340	-2.262	-3.429
	0		0	0	0	0	0		0	0
HoSc	10.097	10.088	10.265	10.268	10.276	10.265	10.269	10.260	10.443	10.433
	3.620	6.142	3.874	4.033	4.044	3.980	3.983	6.079	3.804	6.016



Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.783	2.957	1.931	2.050	2.079	2.008	2.017	2.783	1.718	2.609
	-1.838	-3.185	-1.944	-1.983	-1.965	-1.973	-1.967	-3.296	-2.087	-3.407
	0		0	0	0	0	0		0	
HoSm	10.906	10.902	10.807	10.801	10.802	10.810	10.805	10.803	10.712	10.704
	3.670	5.761	3.733	3.824	3.850	3.785	3.798	5.825	3.930	5.889
	1.353	2.451	1.405	1.490	1.526	1.448	1.468	2.446	1.583	2.440
	-2.318	-3.310	-2.328	-2.334	-2.325	-2.337	-2.331	-3.380	-2.348	-3.449
	0		0	0	0	0	0		0	
HoTb	10.713	10.707	10.681	10.801	10.677	10.676	10.709	10.673	10.643	10.639
	3.882	5.884	3.907	3.894	3.938	3.916	3.914	5.907	3.973	5.930
	1.476	2.472	1.509	1.496	1.532	1.503	1.510	2.460	1.559	2.447
	-2.407	-3.412	-2.398	-2.398	-2.407	-2.414	-2.404	-3.448	-2.415	-3.483
	0.004		0	0	0	0	0		0	
HoTl	10.757	10.726	10.707	10.705	10.706	10.693	10.703	10.686	10.662	10.646
	0.382	1.812	0.871	0.840	0.836	0.856	0.851	3.192	1.307	4.573
	-1.435	-0.893	-1.115	-1.096	-1.119	-1.098	-1.107	0.217	-0.959	1.326
	-1.816	-2.705	-1.986	-1.936	-1.954	-1.954	-1.958	-2.976	-2.265	-3.247
	0		0	0	0	0	0		0	
HoTm	10.51	10.506	10.546	10.502	10.545	10.543	10.534	10.539	10.577	10.572
	4.008	5.997	3.994	4.026	3.958	3.982	3.990	5.982	3.920	5.967
	1.534	2.436	1.527	1.532	1.482	1.513	1.514	2.436	1.456	2.435
	-2.475	-3.561	-2.468	-2.494	-2.477	-2.469	-2.477	-3.547	-2.465	-3.533
	0		24.231	24.050	0	0	12.070		0.076	0
HoV	9.652	9.599	9.932	9.939	9.986	9.882	9.935	9.934	10.308	10.27
	0	3.279	0	0	0.002	0	0.001	4.170	0	5.062
	1.545	2.395	1.522	1.414	1.437	1.406	1.445	2.408	-2.113	2.422
	1.576	-0.875	1.544	1.455	1.435	1.493	1.482	-1.756	-2.105	-2.637
	0		0	0	0	0	0		0	
HoY	10.687	10.68	10.658	10.657	10.655	10.657	10.657	10.655	10.634	10.630
	3.997	5.988	3.988	4.009	4.021	3.997	4.004	5.976	4.001	5.964
	1.627	2.562	1.595	1.624	1.642	1.607	1.617	2.520	1.610	2.477
	-2.370	-3.426	-2.394	-2.385	-2.380	-2.390	-2.388	-3.457	-2.392	-3.488
	0		0	0	0	0	0		0.006	
HoYb	10.682	10.667	10.668	10.538	10.662	10.666	10.634	10.646	10.638	10.626
	3.972	6.017	4.426	4.610	4.494	4.431	4.491	5.996	4.296	5.974
	1.504	2.327	1.534	1.651	1.585	1.537	1.577	2.363	1.644	2.399
	-2.469	-3.691	-2.892	-2.959	-2.909	-2.894	-2.914	-3.634	-2.653	-3.576
	0.033		0.057	0.050	0.050	0.042	0.050		0.040	0
InLa	11.149	11.108	10.872	10.799	10.79	10.856	10.830	10.84	10.587	10.573
	1.778	4.801	1.693	2.134	2.048	1.981	1.964	4.150	1.201	3.499
	-0.070	1.585	-0.105	0.235	0.142	0.158	0.108	0.860	-0.732	0.135
	-1.847	-3.216	-1.797	-1.899	-1.907	-1.824	-1.857	-3.290	-1.933	-3.364
	16.777		26.720	28.699	28.343	27.800	27.891		17.725	
InLu	10.354	10.347	10.342	10.340	10.346	10.348	10.344	10.333	10.335	10.319
	2.507	5.262	2.084	2.159	2.169	2.130	2.136	4.458	1.640	3.653
	-0.051	1.680	-0.362	-0.255	-0.256	-0.293	-0.292	0.923	-0.784	0.167
	-2.557	-3.583	-2.446	-2.413	-2.424	-2.423	-2.427	-3.535	-2.423	-3.487
	20.369		33.011	32.714	32.600	32.912	32.809		29.740	
InMn	9.387	9.352	9.701	9.741	10.673	9.793	9.977	9.670	10.010	9.988

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0	2.382	0	0	0.005	0	0.002	2.538	0	2.693
	0.493	0.813	0.648	0.623	0.678	0.594	0.636	0.346	-19.13	-0.123
	0.629	-1.569	0.677	0.667	0.673	0.659	0.669	-2.192	-19.078	-2.815
	0		0	0	0	0	0		0	
InPm	10.878	10.88	10.709	10.665	10.673	10.701	10.687	10.688	10.516	10.497
	1.966	4.967	1.838	2.153	2.069	2.074	2.034	4.261	1.324	3.555
	-0.263	1.703	-0.332	-0.036	-0.094	-0.120	-0.146	0.939	-0.802	0.175
	-2.228	-3.264	-2.170	-2.188	-2.162	-2.194	-2.179	-3.322	-2.125	-3.380
	18.444		23.849	24.754	23.671	24.673	24.237		0	
InPr	11.038	10.962	10.807	10.749	10.751	10.804	10.778	10.743	10.565	10.524
	1.795	4.936	1.731	2.118	2.016	1.993	1.965	4.240	1.192	3.544
	-0.348	1.706	-0.348	-0.002	-0.075	-0.102	-0.132	0.941	-0.843	0.176
	-2.143	-3.231	-2.079	-2.120	-2.090	-2.095	-2.096	-3.300	-2.035	-3.369
	0		0	0	0	0	0		0	
InSc	10.012	10.013	10.116	10.114	10.129	10.118	10.120	10.110	10.215	10.208
	2.921	5.366	2.398	2.450	2.464	2.412	2.431	4.527	1.880	3.688
	1.024	2.201	0.551	0.655	0.660	0.593	0.615	1.271	-0.061	0.341
	-1.897	-3.165	-1.848	-1.795	-1.804	-1.819	-1.817	-3.256	-1.941	-3.347
	13.051		24.423	24.249	24.236	24.351	24.315		26.877	
InSm	10.823	10.827	10.662	10.634	10.645	10.664	10.652	10.653	10.497	10.479
	2.023	4.985	1.880	2.151	2.074	2.081	2.047	4.273	1.383	3.561
	-0.236	1.695	-0.327	-0.059	-0.112	-0.137	-0.159	0.934	-0.789	0.172
	-2.259	-3.290	-2.206	-2.209	-2.185	-2.218	-2.205	-3.340	-2.171	-3.389
	21.285		33.206	33.482	32.937	33.547	33.293		25.197	0
InTb	10.635	10.632	10.527	10.514	10.520	10.527	10.522	10.523	10.431	10.414
	2.222	5.107	2.001	2.176	2.138	2.134	2.113	4.354	1.528	3.602
	-0.151	1.716	-0.319	-0.115	-0.143	-0.170	-0.187	0.947	-0.764	0.179
	-2.373	-3.392	-2.320	-2.291	-2.28	-2.304	-2.299	-3.408	-2.291	-3.423
	0		0	0	0	0	0		0	
InTl	10.631	10.651	10.518	10.514	10.519	10.516	10.517	10.536	10.416	10.421
	0.001	1.036	0.042	0.001	0.009	0.021	0.019	1.640	0.241	2.244
	-1.759	-1.650	-1.874	-1.891	-1.868	-1.886	-1.88	-1.297	-1.811	-0.944
	-1.759	-2.685	-1.915	-1.891	-1.876	-1.906	-1.897	-2.936	-2.052	-3.187
	0		0	0	0	0	0		0	
InTm	10.435	10.431	10.296	10.318	10.393	10.393	10.350	10.389	10.353	10.347
	2.412	5.221	2.208	2.179	2.164	2.141	2.173	4.430	1.618	3.639
	-0.087	1.680	-0.250	-0.271	-0.216	-0.248	-0.247	0.924	-0.772	0.167
	-2.499	-3.541	-2.458	-2.449	-2.379	-2.388	-2.419	-3.507	-2.39	-3.473
	12.831		24.311	24.384	23.935	24.088	24.179		26.646	
InV	10.614	9.524	10.819	9.893	10.166	9.976	10.214	9.784	10.103	10.045
	0	2.503	0	0	0	0	0	2.618	0	2.733
	1.619	1.639	1.235	1.378	1.221	1.320	1.289	0.896	0.973	0.153
	1.650	-0.856	1.249	1.420	1.239	1.356	1.316	-1.717	1.041	-2.578
	9.287		18.847	22.128	23.215	22.522	21.678		25.275	
InY	9.604	10.605	10.514	10.506	10.501	10.509	10.508	10.505	10.414	10.405
	2.340	5.212	2.059	2.218	2.200	2.184	2.166	4.424	1.600	3.636
	-0.010	1.806	-0.219	-0.025	-0.042	-0.074	-0.090	1.008	-0.682	0.209
	-2.350	-3.406	-2.278	-2.242	-2.242	-2.258	-2.255	-3.417	-2.281	-3.428

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0		0	0	0	0	0		0	
InYb	10.545	10.592	10.477	10.449	10.457	10.479	10.466	10.496	10.382	10.401
	3.355	5.241	2.558	2.724	2.671	2.651	2.651	4.444	1.707	3.646
	0.033	1.570	-0.432	-0.300	-0.334	-0.369	-0.359	0.850	-0.968	0.130
	-3.323	-3.671	-2.990	-3.023	-3.005	-3.019	-3.010	-3.594	-2.675	-3.516
	3.237		4.562	4.598	4.519	4.540	4.555		3.430	
LaLu	10.619	10.614	10.777	10.773	×	×	10.775	10.868	11.148	11.122
	3.859	5.913	3.761	3.599	×	×	3.680	5.759	2.955	5.606
	1.776	2.405	1.752	1.584	×	×	1.668	2.373	1.044	2.342
	-2.083	-3.509	-2.010	-2.015	×	×	-2.013	-3.387	-1.911	-3.264
	21.198		35.043	35.746	×	×	35.396		28.273	
LaMn	10.006	9.620	10.675	10.541	10.325	10.615	10.539	10.205	0	10.790
	0	3.033	0	0	0	0	0	3.839	0	4.646
	0.816	1.538	0.457	0.397	0.660	0.676	0.548	1.796	0	2.053
	0.858	-1.495	0.473	0.427	0.677	0.696	0.569	-2.044	0	-2.593
	0		0	0	0	0	0		0	
LaPm	11.149	11.147	11.236	11.242	11.242	11.233	11.239	11.223	11.322	11.299
	3.873	5.617	3.775	3.646	3.576	3.714	3.678	5.562	3.380	5.507
	1.735	2.428	1.679	1.574	1.521	1.624	1.600	2.389	1.415	2.350
	-2.138	-3.190	-2.096	-2.072	-2.055	-2.091	-2.079	-3.174	-1.965	-3.158
	0		0	0	0	0	0		0	
LaPr	11.313	11.229	11.344	11.242	11.349	11.345	11.32	11.278	11.377	11.327
	3.788	5.587	3.752	3.633	3.579	3.695	3.665	5.542	3.437	5.497
	1.649	2.431	1.642	1.553	1.518	1.596	1.578	2.391	1.463	2.350
	-2.139	-3.157	-2.111	-2.08	-2.062	-2.099	-2.088	-3.152	-1.974	-3.147
	0		0	0	0	0	0		0	
LaSc	10.308	10.280	10.634	10.645	10.678	10.615	10.643	10.645	11.040	11.010
	3.229	6.017	3.576	3.526	3.337	3.631	3.518	5.828	2.778	5.640
	1.626	2.926	1.906	1.766	1.660	1.846	1.795	2.721	1.021	2.516
	-1.603	-3.091	-1.671	-1.760	-1.677	-1.786	-1.724	-3.108	-1.758	-3.125
	13.056		25.869	26.163	25.618	26.089	25.935		26.414	
LaSm	11.094	11.094	11.196	11.204	11.206	11.195	11.201	11.188	11.309	11.282
	3.877	5.636	3.777	3.634	3.564	3.709	3.671	5.575	3.351	5.513
	1.742	2.420	1.688	1.568	1.515	1.623	1.599	2.384	1.391	2.347
	-2.135	-3.216	-2.090	-2.067	-2.050	-2.086	-2.074	-3.191	-1.96	-3.167
	31.851		42.713	42.208	41.458	42.574	42.238		28.524	
LaTb	10.903	10.900	11.067	11.077	11.077	11.064	11.072	11.058	11.243	11.217
	3.922	5.758	3.758	3.607	3.512	3.690	3.642	5.656	3.237	5.554
	1.799	2.441	1.702	1.566	1.494	1.628	1.598	2.397	1.292	2.354
	-2.124	-3.318	-2.056	-2.042	-2.019	-2.063	-2.045	-3.259	-1.945	-3.201
	0		0	0	0	0	0		0	
LaTl	10.963	10.919	11.098	11.137	11.135	11.104	11.119	11.071	11.279	11.223
	0.366	1.687	0.834	0.924	0.946	0.892	0.899	2.942	1.052	4.197
	-1.243	-0.925	-0.873	-0.756	-0.736	-0.818	-0.796	0.154	-0.731	1.232
	-1.609	-2.611	-1.706	-1.68	-1.682	-1.709	-1.695	-2.788	-1.783	-2.965
	0		0	0	0	0	0		0	
LaTm	10.698	10.698	10.878	10.879	10.945	10.919	10.906	10.924	11.175	11.150
	3.886	5.871	3.747	3.587	3.415	3.642	3.598	5.732	3.048	5.592
	1.791	2.405	1.721	1.566	1.449	1.618	1.589	2.373	1.126	2.342

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	-2.096	-3.467	-2.027	-2.021	-1.967	-2.025	-2.010	-3.359	-1.922	-3.250
	14.857		27.537	27.747	27.189	27.320	27.448		27.894	
LaV	10.049	9.791	10.225	10.338	10.337	10.302	10.301	10.319	10.795	10.847
	0	3.154	0.016	0.006	0	0.013	0.009	3.920	0	4.686
	1.470	2.364	1.470	1.377	1.337	1.322	1.377	2.346	1.077	2.328
	1.516	-0.781	1.454	1.372	1.352	1.310	1.372	-1.568	1.136	-2.355
	11.974		24.301	24.092	23.14	24.722	24.064		22.988	
LaY	10.878	10.873	11.051	10.977	11.062	11.046	11.034	11.040	11.238	11.208
	3.999	5.862	3.791	3.680	3.532	3.712	3.679	5.726	3.242	5.589
	1.914	2.531	1.758	1.635	1.538	1.674	1.652	2.458	1.312	2.384
	-2.085	-3.332	-2.034	-2.046	-1.994	-2.039	-2.029	-3.269	-1.930	-3.205
	0		0	0	0	0	0		0	
LaYb	10.860	10.859	11.049	10.912	11.051	11.048	11.015	11.031	11.233	11.203
	4.603	5.892	4.186	4.067	3.958	4.095	4.077	5.745	3.542	5.599
	2.113	2.295	1.872	1.780	1.703	1.777	1.783	2.300	1.484	2.305
	-2.491	-3.597	-2.314	-2.287	-2.256	-2.318	-2.294	-3.445	-2.059	-3.294
	1.889		0	0.916	0.878	0	0.449		1.615	
LuMn	9.380	9.366	9.670	9.681	9.712	9.672	9.684	9.697	0	10.029
	0	3.187	0	0	0	0	0	4.147	0	5.107
	0.540	1.570	0.675	0.640	0.663	0.655	0.659	1.858	0	2.147
	0.556	-1.618	0.738	0.664	0.688	0.673	0.691	-2.289	0	-2.960
	0		0	0	0	0	0		0	
LuPm	10.896	10.894	10.723	10.610	10.709	10.721	10.691	10.716	10.542	10.538
	3.409	5.771	3.539	3.862	3.813	3.675	3.723	5.870	3.913	5.968
	1.128	2.459	1.251	1.508	1.514	1.359	1.408	2.451	1.570	2.444
	-2.281	-3.312	-2.289	-2.355	-2.300	-2.317	-2.316	-3.419	-2.344	-3.525
	0		0	0	0	0	0		0	
LuPr	11.067	10.975	10.833	10.717	10.803	10.827	10.795	10.770	10.595	10.565
	3.152	5.741	3.306	3.720	3.704	3.505	3.559	5.849	3.807	5.958
	0.947	2.462	1.129	1.451	1.482	1.281	1.336	2.453	1.543	2.445
	-2.205	-3.279	-2.177	-2.269	-2.222	-2.224	-2.223	-3.397	-2.265	-3.514
	0		0	0	0	0	0		0	
LuSc	10.029	10.027	10.140	10.058	10.146	10.141	10.122	10.138	10.258	10.249
	3.721	6.170	3.988	4.211	4.197	4.078	4.119	6.136	4.050	6.101
	1.820	2.957	1.992	2.162	2.216	2.076	2.112	2.784	1.902	2.610
	-1.901	-3.213	-1.997	-2.050	-1.982	-2.003	-2.008	-3.353	-2.149	-3.492
	22.382		35.520	36.168	35.650	35.602	35.735		31.916	
LuSm	10.847	10.840	10.685	10.622	10.675	10.683	10.667	10.680	10.527	10.520
	2.432	5.789	3.607	3.852	3.837	3.722	3.755	5.882	3.938	5.974
	0.141	2.452	1.281	1.483	1.509	1.374	1.412	2.446	1.568	2.441
	-2.292	-3.338	-2.327	-2.369	-2.328	-2.349	-2.344	-3.436	-2.371	-3.534
	0		0	0	0	0	0		0	
LuTb	10.654	10.646	10.557	10.553	10.553	10.559	10.556	10.551	10.457	10.456
	0.711	5.912	3.832	3.927	3.956	3.889	3.901	5.964	4.033	6.015
	-1.679	2.472	1.383	1.482	1.523	1.437	1.457	2.460	1.573	2.448
	-2.389	-3.440	-2.450	-2.445	-2.433	-2.453	-2.446	-3.504	-2.461	-3.568
	0		0	0	0	0	0		0	
LuTl	10.694	10.665	10.581	10.571	10.574	10.565	10.573	10.563	10.478	10.462
	0	1.840	0.885	0.805	0.796	0.844	0.833	3.249	1.376	4.658

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	-16.554	-0.893	-1.158	-1.181	-1.208	-1.167	-1.179	0.217	-0.942	1.327
	-16.912	-2.733	-2.042	-1.986	-2.004	-2.010	-2.011	-3.032	-2.318	-3.332
	0		0	0	0	0	0		0	
LuTm	10.449	10.444	10.419	10.377	10.421	10.421	10.410	10.416	10.392	10.388
	3.960	6.025	3.987	4.076	4.020	3.994	4.020	6.039	4.052	6.053
	1.440	2.436	1.440	1.510	1.482	1.453	1.472	2.436	1.509	2.436
	-2.521	-3.589	-2.547	-2.566	-2.538	-2.541	-2.548	-3.603	-2.543	-3.617
	8.125		13.093	13.066	35.598	35.627	24.346		32.056	
LuV	9.581	9.538	9.827	9.729	9.884	9.802	9.811	9.812	10.133	10.086
	0	3.308	0	0	0	0	0	4.227	0	5.147
	1.592	2.395	1.542	1.449	1.425	1.440	1.464	2.409	1.283	2.422
	1.606	-0.904	1.584	1.476	1.435	1.503	1.500	-1.813	1.289	-2.722
	16.323		29.281	30.651	30.737	30.275	30.236		25.683	
LuY	10.625	10.619	10.535	10.531	10.532	10.537	10.534	10.533	10.447	10.447
	0	6.016	3.929	4.029	4.052	3.980	3.998	6.033	4.081	6.050
	-9.843	2.562	1.503	1.608	1.647	1.559	1.580	2.520	1.637	2.478
	-13.697	-3.454	-2.426	-2.421	-2.405	-2.422	-2.419	-3.513	-2.444	-3.572
	0		0	0	0	0	0		0	
LuYb	10.612	10.606	10.528	10.528	10.529	10.528	10.529	10.524	10.442	10.442
	0	6.046	4.424	4.540	4.583	4.483	4.508	6.053	4.361	6.060
	-4.441	2.327	1.434	1.520	1.560	1.477	1.498	2.363	1.622	2.400
	-8.383	-3.719	-2.99	-3.020	-3.023	-3.007	-3.010	-3.690	-2.740	-3.661
	0		1.272	1.416	1.543	1.317	1.387		1.286	
MnPm	10.596	10.562	10.120	9.777	9.822	10.147	9.967	10.053	9.868	9.544
	0	4.811	0	0	0.004	0.025	0.008	3.950	0	3.088
	0.358	2.170	0.708	0.646	0.730	0.630	0.679	1.874	0.845	1.577
	0.380	-2.641	0.766	0.691	0.726	0.606	0.698	-2.076	0.853	-1.511
	1.124		10.329	13.404	13.907	13.539	12.795		17.292	
MnPr	10.747	10.644	10.237	9.933	9.952	10.280	10.101	10.107	9.964	9.571
	0	4.781	0	0	0	0	0	3.929	0	3.078
	0.396	2.173	0.712	0.670	0.691	0.676	0.688	1.876	0.838	1.578
	0.418	-2.608	0.745	0.690	0.695	0.710	0.710	-2.054	0.856	-1.500
	1.662		8.417	11.806	12.208	14.206	11.660		17.605	0
MnSc	9.739	9.695	9.477	9.461	9.460	9.477	9.469	9.475	9.274	9.255
	0	5.210	0	0.006	0	0	0.002	4.216	0	3.221
	0.483	2.669	0.600	0.649	0.661	0.620	0.633	2.206	0.514	1.743
	0.513	-2.542	0.603	0.644	0.684	0.638	0.643	-2.010	0.531	-1.478
	4.239		13.459	13.899	13.633	13.735	13.682		25.538	
MnSm	10.531	10.509	10.027	9.746	9.799	10.106	9.920	10.017	9.856	9.526
	0	4.829	0	0	0	0.028	0.007	3.962	0	3.094
	-13.088	2.163	0.583	0.644	0.724	0.632	0.646	1.869	0.852	1.575
	-13.088	-2.667	0.597	0.688	0.732	0.605	0.656	-2.093	0.863	-1.520
	0		10.437	13.798	14.116	13.821	13.043		20.059	
MnTb	10.357	10.315	9.897	9.683	9.705	10.091	9.844	9.888	9.469	9.461
	0	4.952	0	0	0	0	0	4.044	0	3.135
	0.285	2.183	0.576	0.627	0.688	0.703	0.649	1.883	0.543	1.582
	0.312	-2.769	0.598	0.675	0.695	0.710	0.670	-2.161	0.560	-1.554
	2.332		9.905	14.892	14.445	15.757	13.750		11.544	
MnTl	10.368	10.333	11.276	10.338	11.49	12.031	11.284	9.900	10.494	9.467

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0	0.880	0	0	0.027	0	0.007	1.329	0	1.778
	0.178	-1.182	0.833	0.702	0.914	0.858	0.827	-0.361	0.784	0.460
	0.290	-2.062	0.851	0.723	0.888	0.884	0.837	-1.690	0.850	-1.318
	15.852		27.659	24.243	28.419	27.787	27.027		25.971	
MnTm	10.164	10.113	9.762	9.615	9.635	9.810	9.706	9.753	9.398	9.394
	0	5.065	0	0	0	0	0	4.119	0	3.173
	0.205	2.148	0.585	0.627	0.673	0.662	0.637	1.859	0.551	1.570
	0.232	-2.918	0.605	0.669	0.681	0.699	0.664	-2.261	0.551	-1.604
	2.800		11.537	12.655	12.252	11.993	12.109		23.858	
MnV	9.204	9.206	9.145	9.166	9.151	9.133	9.149	9.149	9.105	9.092
	0	2.348	0	0	0	0	0	2.307	0	2.267
	1.202	2.107	0.889	0.849	0.770	0.850	0.840	1.831	0.609	1.556
	1.261	-0.232	0.937	0.851	0.791	0.863	0.861	-0.470	0.662	-0.708
	7.253		17.153	18.084	18.087	18.344	17.917		28.725	
MnY	10.359	10.288	9.878	9.813	9.702	9.942	9.834	9.870	9.453	9.452
	0	5.056	0	0	0	0.001	0.001	4.113	0	3.170
	0.274	2.274	0.578	0.667	0.687	0.705	0.66	1.943	0.551	1.612
	0.310	-2.783	0.597	0.683	0.688	0.704	0.668	-2.171	0.590	-1.559
	2.816		10.269	13.755	13.951	12.784	12.690		13.073	
MnYb	10.038	10.274	9.750	9.564	9.545	9.796	9.664	9.861	9.719	9.448
	0	5.086	0	0	0.009	0	0.003	4.133	0	3.180
	-0.622	2.038	0.469	0.401	0.496	0.421	0.447	1.786	0.799	1.533
	-0.473	-3.048	0.504	0.450	0.488	0.430	0.468	-2.347	0.837	-1.647
	21.706		35.511	36.583	36.399	36.139	36.158		38.624	
PmPr	11.233	11.153	11.181	11.179	11.177	11.181	11.180	11.126	11.123	11.099
	3.637	5.642	3.667	3.702	3.718	3.682	3.693	5.652	3.776	5.662
	1.417	2.470	1.444	1.479	1.497	1.458	1.470	2.469	1.544	2.468
	-2.221	-3.173	-2.223	-2.223	-2.221	-2.224	-2.223	-3.184	-2.233	-3.195
	0		0	0	0	0	0		0	0
PmSc	10.217	10.204	10.489	10.492	10.510	10.477	10.492	10.493	10.786	10.782
	3.418	6.072	3.675	3.785	3.665	3.812	3.735	5.939	3.247	5.806
	1.719	2.965	1.869	1.889	1.813	1.922	1.874	2.799	1.274	2.633
	-1.699	-3.107	-1.806	-1.896	-1.852	-1.891	-1.862	-3.140	-1.974	-3.173
	12.497		24.678	25.026	24.795	24.901	24.85		26.933	
PmSm	11.017	11.018	11.039	11.034	11.036	11.036	11.037	11.036	11.057	11.054
	3.803	5.691	3.792	3.787	3.778	3.789	3.787	5.685	3.760	5.679
	1.530	2.459	1.523	1.513	1.504	1.518	1.515	2.462	1.492	2.464
	-2.274	-3.232	-2.269	-2.275	-2.275	-2.272	-2.273	-3.223	-2.269	-3.215
	29.924		43.061	43.117	43.141	43.092	43.103		5.316	
PmTb	10.829	10.824	10.908	10.911	10.91	10.907	10.909	10.906	10.992	10.989
	3.894	5.813	3.843	3.805	3.779	3.827	3.814	5.766	3.683	5.719
	1.583	2.480	1.558	1.503	1.473	1.533	1.517	2.476	1.393	2.471
	-2.312	-3.334	-2.285	-2.302	-2.306	-2.295	-2.297	-3.291	-2.290	-3.249
	0		0	0	0	0	0		0	
PmTl	10.890	10.843	10.942	10.956	10.948	10.934	10.945	10.919	11.020	10.995
	0.356	1.742	0.813	0.878	0.878	0.854	0.856	3.052	1.161	4.362
	-1.383	-0.885	-1.066	-0.972	-0.987	-1.004	-1.008	0.233	-0.990	1.350
	-1.739	-2.627	-1.878	-1.850	-1.865	-1.858	-1.863	-2.820	-2.150	-3.013

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	0		0	0	0	0	0		0	
PmTm	10.626	10.622	10.773	10.688	10.775	10.770	10.752	10.772	10.920	10.922
	3.915	5.927	3.835	3.862	3.709	3.816	3.806	5.842	3.500	5.757
	1.579	2.444	1.555	1.512	1.392	1.516	1.494	2.452	1.211	2.459
	-2.336	-3.483	-2.281	-2.351	-2.318	-2.300	-2.313	-3.391	-2.290	-3.298
	13.862		25.700	26.151	25.866	25.816	25.883		27.872	
PmV	9.896	9.715	10.093	10.332	10.200	10.046	10.168	10.167	10.574	10.619
	0	3.209	0	0	0	0	0	4.03	0.011	4.851
	1.505	2.403	1.509	1.155	1.396	1.369	1.358	2.424	1.231	2.446
	1.550	-0.797	1.525	1.175	1.415	1.400	1.379	-1.600	1.220	-2.403
	10.503		22.159	23.337	21.990	22.493	22.495		23.131	
PmY	10.799	10.797	10.888	10.891	10.890	10.886	10.889	10.888	10.979	10.980
	3.997	5.918	3.899	3.849	3.819	3.877	3.861	5.836	3.699	5.754
	1.726	2.570	1.644	1.579	1.548	1.613	1.596	2.536	1.428	2.501
	-2.271	-3.348	-2.256	-2.270	-2.272	-2.265	-2.266	-3.301	-2.272	-3.253
	0		0	0	0	0	0		0	0
PmYb	10.806	10.783	10.910	10.907	10.904	10.910	10.908	10.879	10.994	10.975
	3.990	5.947	4.296	4.236	4.239	4.252	4.256	5.856	4.013	5.764
	1.580	2.335	1.608	1.538	1.539	1.562	1.562	2.379	1.523	2.423
	-2.410	-3.613	-2.689	-2.699	-2.701	-2.691	-2.695	-3.477	-2.490	-3.342
	34.868		1.745	1.881	2.014	1.793	1.858		2.247	
PrSc	10.278	10.232	10.584	10.592	10.624	10.569	10.593	10.548	10.946	10.864
	3.336	6.062	3.615	3.684	3.485	3.762	3.637	5.919	2.958	5.775
	1.698	2.966	1.883	1.825	1.691	1.905	1.826	2.801	1.039	2.636
	-1.639	-3.096	-1.732	-1.860	-1.794	-1.858	-1.811	-3.118	-1.920	-3.140
	10.833		22.632	23.005	22.627	22.880	22.786		25.034	
PrSm	11.07	11.045	11.145	11.146	11.141	11.142	11.144	11.090	11.217	11.135
	3.784	5.681	3.734	3.697	3.681	3.715	3.707	5.665	3.601	5.648
	1.546	2.460	1.517	1.470	1.449	1.492	1.482	2.464	1.379	2.467
	-2.238	-3.221	-2.218	-2.228	-2.232	-2.224	-2.226	-3.201	-2.222	-3.182
	25.854		37.367	37.582	37.58	37.492	37.506		28.623	
PrTb	10.881	10.851	11.015	11.017	11.018	11.011	11.016	10.961	11.154	11.071
	3.829	5.803	3.751	3.694	3.640	3.732	3.705	5.746	3.474	5.689
	1.574	2.481	1.532	1.453	1.401	1.498	1.471	2.478	1.251	2.474
	-2.255	-3.323	-2.219	-2.241	-2.240	-2.234	-2.234	-3.269	-2.224	-3.216
	0		0	0	0	0	0		0	
PrTl	10.949	10.870	11.049	11.074	11.067	11.048	11.060	10.973	11.185	11.077
	0.303	1.732	0.777	0.881	0.878	0.833	0.843	3.032	1.066	4.332
	-1.387	-0.884	-1.058	-0.939	-0.952	-0.984	-0.984	0.235	-1.007	1.353
	-1.689	-2.616	-1.835	-1.820	-1.83	-1.817	-1.826	-2.798	-2.072	-2.980
	0		0	0	0	0	0		0	
PrTm	10.681	10.649	10.781	10.785	10.885	10.870	10.831	10.826	11.088	11.003
	3.815	5.917	3.831	3.742	3.548	3.714	3.709	5.822	3.254	5.727
	1.553	2.445	1.591	1.467	1.316	1.487	1.466	2.454	1.040	2.462
	-2.263	-3.472	-2.240	-2.275	-2.233	-2.228	-2.244	-3.369	-2.214	-3.265
	12.351		23.942	24.222	23.919	23.902	23.996		26.220	
PrV	10.031	9.743	10.06	10.206	10.292	10.240	10.200	10.222	10.710	10.701
	0	3.199	0	0.001	0	0	0.001	4.010	0	4.821
	1.488	2.404	1.461	1.386	1.369	1.425	1.411	2.426	1.131	2.449

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.521	-0.786	1.466	1.386	1.381	1.446	1.420	-1.578	1.131	-2.370
	9.815		21.048	21.296	20.226	20.962	20.883		21.864	
PrY	10.847	10.824	10.997	10.998	10.999	10.991	10.997	10.943	11.143	11.062
	3.932	5.907	3.796	3.724	3.670	3.771	3.741	5.816	3.479	5.724
	1.722	2.571	1.609	1.517	1.464	1.567	1.540	2.538	1.274	2.504
	-2.211	-3.337	-2.187	-2.208	-2.206	-2.204	-2.202	-3.278	-2.206	-3.220
	0		0	0	0	0	0		0	
PrYb	10.865	10.811	11.02	11.017	11.013	11.014	11.016	10.934	11.168	11.057
	4.040	5.937	4.199	4.096	4.091	4.139	4.132	5.835	3.817	5.734
	1.563	2.336	1.592	1.486	1.472	1.532	1.521	2.381	1.401	2.426
	-2.478	-3.602	-2.607	-2.610	-2.620	-2.607	-2.611	-3.455	-2.417	-3.309
	27.104		38.771	37.020	38.317	36.047	37.539		26.634	0
ScSm	10.731	10.729	10.471	10.426	10.426	10.462	10.447	10.458	10.199	10.187
	3.337	5.824	3.532	3.818	3.829	3.725	3.726	5.951	3.449	6.078
	1.348	2.626	1.747	1.909	1.928	1.852	1.859	2.794	1.727	2.963
	-1.989	-3.199	-1.785	-1.910	-1.902	-1.874	-1.868	-3.157	-1.722	-3.116
	0		0	0	0	0	0		0	
ScTb	10.542	10.535	10.339	10.316	10.318	10.337	10.328	10.328	10.126	10.122
	3.653	5.947	3.839	3.958	3.925	3.945	3.917	6.033	3.561	6.119
	1.598	2.646	1.955	1.997	1.975	2.003	1.983	2.808	1.759	2.969
	-2.056	-3.301	-1.885	-1.961	-1.951	-1.943	-1.935	-3.225	-1.802	-3.150
	0		0	0	0	0	0		0	
ScTl	10.564	10.554	10.356	10.331	10.334	10.336	10.340	10.341	10.129	10.128
	0.514	1.875	1.108	0.967	0.935	1.045	1.014	3.318	1.616	4.762
	-0.888	-0.719	-0.360	-0.445	-0.496	-0.404	-0.427	0.565	-0.034	1.848
	-1.402	-2.594	-1.467	-1.412	-1.431	-1.448	-1.440	-2.754	-1.65	-2.914
	0		0	0	0	0	0		0	
ScTm	10.339	10.333	10.201	10.143	10.191	10.201	10.184	10.194	10.060	10.055
	3.946	6.060	4.087	2.790	4.039	4.128	3.761	6.108	3.676	6.156
	1.825	2.610	2.148	1.331	2.044	2.153	1.919	2.784	1.802	2.958
	-2.121	-3.450	-1.939	-1.460	-1.995	-1.976	-1.843	-3.325	-1.875	-3.199
	28.311		37.053	0	36.956	37.541	27.888		23.230	
ScV	9.456	9.426	9.605	9.619	9.638	9.622	9.621	9.589	9.781	9.752
	0	3.342	0	0	0	0.006	0.002	4.296	0	5.251
	1.542	2.569	1.575	1.486	1.385	1.43	1.469	2.756	1.475	2.944
	1.564	-0.764	1.660	1.529	1.405	1.425	1.505	-1.534	1.496	-2.304
	0		0	0	0	0	0		0	
ScY	10.512	10.508	10.315	10.297	10.300	10.315	10.307	10.310	10.114	10.113
	3.758	6.051	3.938	4.013	3.956	4.018	3.982	6.102	3.589	6.153
	1.708	2.736	2.024	2.039	1.998	2.065	2.032	2.868	1.777	3.000
	-2.050	-3.315	-1.914	-1.974	-1.958	-1.954	-1.950	-3.235	-1.812	-3.154
	0		0	0	0	0	0		0	
ScYb	10.466	10.494	10.275	10.267	10.267	10.275	10.271	10.301	10.085	10.108
	4.581	6.080	4.487	4.676	4.691	4.616	4.618	6.122	3.702	6.163
	1.912	2.501	2.275	2.378	2.387	2.348	2.347	2.711	1.741	2.921
	-2.670	-3.580	-2.213	-2.298	-2.304	-2.269	-2.271	-3.411	-1.961	-3.243
	0.099		0.090	0.102	0.108	0.093	0.098		0.051	
SmTb	10.808	10.806	10.872	10.875	10.875	10.872	10.874	10.871	10.940	10.936
	3.910	5.820	3.854	3.829	3.809	3.840	3.833	5.779	3.736	5.738



Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	1.578	2.478	1.547	1.507	1.484	1.525	1.516	2.471	1.423	2.464
	-2.333	-3.343	-2.308	-2.323	-2.326	-2.315	-2.318	-3.309	-2.314	-3.275
	0		0	0	0	0	0		0	
SmTl	10.869	10.825	10.907	10.917	10.909	10.898	10.908	10.883	10.962	10.942
	0.369	1.748	0.819	0.869	0.869	0.852	0.853	3.064	1.187	4.381
	-1.389	-0.888	-1.076	-0.993	-1.008	-1.021	-1.025	0.228	-0.985	1.342
	-1.757	-2.635	-1.894	-1.862	-1.877	-1.872	-1.877	-2.837	-2.172	-3.039
	0		0	0	0	0	0		0	
SmTm	10.604	10.604	10.655	10.653	10.740	10.733	10.696	10.736	10.870	10.868
	3.930	5.933	3.961	3.895	3.752	3.843	3.863	5.854	3.578	5.776
	1.571	2.442	1.614	1.517	1.406	1.514	1.513	2.447	1.260	2.452
	-2.360	-3.492	-2.347	-2.378	-2.346	-2.329	-2.350	-3.408	-2.319	-3.324
	17.185		30.119	30.295	29.955	29.891	30.065		29.700	
SmV	9.847	9.698	10.069	10.212	10.170	10.020	10.118	10.132	10.536	10.566
	0	3.215	0	0	0	0	0	4.042	0.003	4.870
	1.527	2.401	1.536	1.381	1.401	1.369	1.422	2.419	1.269	2.438
	1.556	-0.806	1.545	1.406	1.420	1.406	1.445	-1.618	1.267	-2.429
	12.936		25.318	26.101	25.321	25.903	25.661		23.747	
SmY	10.778	10.779	10.852	10.856	10.854	10.850	10.853	10.853	10.927	10.927
	4.009	5.924	3.913	3.876	3.855	3.900	3.886	5.848	3.761	5.773
	1.718	2.568	1.635	1.584	1.562	1.612	1.599	2.531	1.466	2.494
	-2.292	-3.356	-2.279	-2.292	-2.293	-2.288	-2.288	-3.318	-2.295	-3.279
	0		0	0	0	0	0		0	
TmYb	10.786	10.766	10.875	10.873	10.864	10.872	10.871	10.844	10.941	10.922
	3.954	5.953	4.312	4.268	4.276	4.281	4.285	5.868	4.056	5.782
	1.573	2.332	1.592	1.538	1.546	1.557	1.559	2.374	1.542	2.415
	-2.381	-3.622	-2.721	-2.730	-2.730	-2.724	-2.727	-3.495	-2.514	-3.368
	0.144		1.216	2.003	2.781	1.501	1.875		4.216	
TbTl	10.793	10.76	10.776	10.777	10.774	10.765	10.773	10.754	10.769	10.748
	0.377	1.789	0.860	0.854	0.853	0.860	0.857	3.146	1.268	4.503
	-1.421	-0.881	-1.096	-1.056	-1.075	-1.067	-1.074	0.241	-0.967	1.363
	-1.798	-2.669	-1.955	-1.909	-1.928	-1.926	-1.930	-2.905	-2.234	-3.141
	0		0	0	0	0	0		0	
TbTm	10.543	10.540	10.610	10.520	10.613	10.609	10.588	10.607	10.680	10.674
	3.996	5.974	3.962	4.039	3.901	3.945	3.962	5.936	3.824	5.898
	1.559	2.449	1.550	1.567	1.465	1.524	1.527	2.460	1.405	2.472
	-2.438	-3.526	-2.412	-2.473	-2.436	-2.421	-2.436	-3.476	-2.420	-3.426
	9.380		19.835	20.078	19.882	19.859	19.914		26.962	
TbV	9.709	9.633	9.969	9.903	10.047	9.926	9.962	10.002	10.396	10.372
	0	3.256	0	0	0	0	0	4.124	0	4.992
	1.555	2.407	1.490	1.412	1.415	1.389	1.427	2.433	1.320	2.459
	1.558	-0.840	1.542	1.413	1.442	1.462	1.465	-1.686	1.323	-2.531
	6.950		16.979	17.598	17.302	17.421	17.325		22.394	
TbY	10.717	10.714	10.725	10.728	10.726	10.725	10.726	10.723	10.733	10.732
	4.025	5.965	3.983	3.985	3.982	3.984	3.984	5.930	3.946	5.895
	1.675	2.575	1.625	1.626	1.627	1.625	1.626	2.545	1.581	2.514
	-2.350	-3.390	-2.358	-2.359	-2.356	-2.359	-2.358	-3.386	-2.365	-3.381
	32.703		45.977	46.829	3.113	46.405	35.581		2.515	
TbYb	10.717	10.701	10.742	10.737	10.734	10.735	10.737	10.714	10.741	10.728

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	PBE <sup>1st</sup>	PBE <sup>2nd</sup>	PBE <sup>3rd</sup>	PBE <sup>4th</sup>	PBE <sup>aver.</sup>	interp. HSE	PBE	interp. HSE
	4.049	5.994	4.390	4.407	4.429	4.399	4.407	5.950	4.233	5.905
	1.549	2.339	1.564	-1.526	1.584	1.561	0.796	2.387	1.627	2.436
	-2.501	-3.656	-2.827	-5.932	-2.846	-2.838	-3.611	-3.563	-2.607	-3.470
	9.565		16.191	16.309	16.451	16.230	16.295		16.660	
TlTm	10.558	10.546	10.631	10.526	10.643	10.63	10.608	10.619	10.719	10.693
	1.348	4.616	0.796	0.915	0.844	0.814	0.843	3.221	0.367	1.826
	-0.948	1.327	-1.183	-1.081	1.363	-1.169	-0.518	0.218	-1.464	-0.893
	-2.296	-3.290	-1.979	-1.995	1.325	-1.983	-1.158	-3.004	-1.831	-2.719
	8.282		18.573	18.620	18.480	18.560	18.558		27.376	
TlV	10.609	9.639	10.821	11.096	12.23	11.542	11.423	10.015	10.481	10.391
	0	1.899	1.271	1.673	1.351	2.156	1.613	1.410	0	0.921
	1.319	1.286	0.735	1.338	1.236	-0.048	0.816	0.190	0.422	-0.907
	1.432	-0.604	-0.537	-0.335	-0.114	-2.203	-0.798	-1.214	0.648	-1.824
	14.005		30.882	31.554	33.159	32.632	32.057		29.766	
TlY	10.735	10.721	10.750	10.743	10.755	10.748	10.749	10.736	10.781	10.751
	1.332	4.607	0.856	0.889	0.898	0.884	0.882	3.215	0.400	1.823
	-0.849	1.453	-1.038	-0.973	1.643	-0.996	-0.341	0.302	-1.362	-0.851
	-2.180	-3.155	-1.893	-1.862	-2.396	-1.879	-2.008	-2.914	-1.761	-2.674
	21.179		32.609	32.047	31.769	32.486	32.228		25.895	
TlYb	10.669	10.707	10.686	10.683	10.687	10.705	10.691	10.727	10.728	10.747
	2.247	4.634	1.280	1.377	1.383	1.343	1.346	3.235	0.458	1.833
	-0.839	1.217	-1.273	-1.137	-1.147	-1.201	-1.190	0.144	-1.626	-0.930
	-3.086	-3.420	-2.553	-2.514	-2.530	-2.543	-2.535	-3.091	-2.084	-2.762
	11.023		19.303	19.389	19.311	19.359	19.340		20.228	
TmV	9.622	9.566	9.881	9.772	9.927	9.837	9.855	9.868	10.209	10.170
	0	3.294	0	0	0.038	0	0.010	4.200	0	5.105
	1.556	2.395	1.531	1.539	-1.140	1.422	0.838	2.409	1.297	2.423
	1.599	-0.890	1.565	1.574	-1.983	1.494	0.663	-1.785	1.305	-2.680
	0		0	0	0	0	0		0	
TmY	10.643	10.647	10.595	10.511	10.587	10.589	10.571	10.589	10.532	10.531
	3.948	6.002	3.956	4.054	4.038	3.992	4.010	6.005	4.040	6.008
	1.564	2.563	1.543	1.600	-0.98	1.581	0.936	2.521	1.621	2.479
	-2.384	-3.440	-2.413	-2.454	-1.878	-2.411	-2.289	-3.485	-2.420	-3.530
	0		0	0.116	0	0	0.029		0	
TmYb	10.642	10.634	10.590	10.490	10.591	10.591	10.566	10.580	10.528	10.526
	3.963	6.032	4.420	4.545	4.545	4.456	4.492	6.025	4.332	6.018
	1.454	2.327	1.477	1.561	1.571	1.501	1.528	2.364	1.630	2.400
	-2.509	-3.705	-2.944	-2.985	-2.975	-2.955	-2.965	-3.662	-2.702	-3.619
	0.046		0.052	0.063	0.061	0.053	0.057		0.046	
VY	10.372	10.345	10.052	9.877	9.902	10.059	9.973	9.984	9.693	9.624
	0	5.096	0	0	0	0	0	4.194	0	3.291
	1.341	2.549	1.461	1.410	1.403	1.423	1.425	2.493	1.558	2.438
	1.346	-2.545	1.484	1.421	1.478	1.442	1.457	-1.695	1.567	-0.845
	0		0	0	0	0	0		0	
VYb	10.140	10.331	9.894	9.848	9.743	9.881	9.842	9.975	9.612	9.619
	0	5.126	0	0	0.015	0.006	0.006	4.213	0.008	3.300
	0.293	2.313	1.317	1.203	1.246	1.207	1.244	2.336	1.476	2.359
	0.387	-2.810	1.356	1.276	1.231	1.201	1.266	-1.872	1.468	-0.933

Table1 Continued

XY	$(X_{0.25}Y_{0.75})_2O_3$		$(X_{0.5}Y_{0.5})_2O_3$					$(X_{0.75}Y_{0.25})_2O_3$		
	PBE	interp. HSE	$PBE^{1st}$	$PBE^{2nd}$	$PBE^{3rd}$	$PBE^{4th}$	$PBE^{aver.}$	interp. HSE	PBE	interp. HSE
	10.666		7.064	6.810	6.815	6.869	6.889		1.352	
YYb	10.705	10.692	10.718	10.712	10.712	10.717	10.715	10.696	10.711	10.701
	4.132	6.029	4.478	4.501	4.531	4.474	4.496	6.019	4.367	6.009
	1.634	2.369	1.710	1.713	1.736	1.701	1.715	2.448	1.808	2.526
	-2.499	-3.660	-2.768	-2.788	-2.796	-2.774	-2.782	-3.572	-2.559	-3.483
	9.083		14.938	14.995	15.107	14.948	14.997		14.774	