Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Full *in silico* DFT characterization of lanthanum and yttrium based oxynitride semiconductors for solar fuels

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Author Contributions

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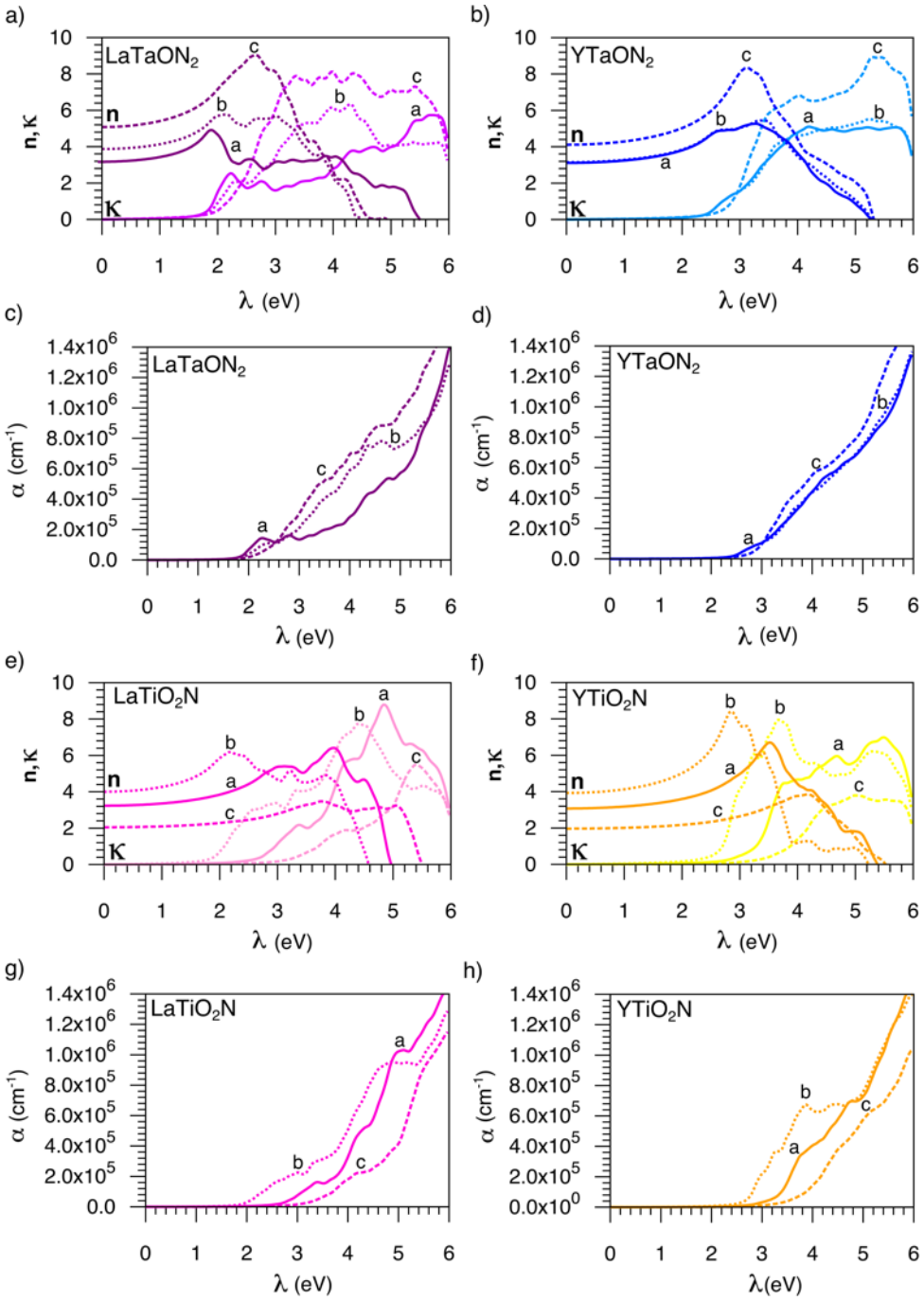

Fig. S1. Theoretical refractive index *n* and extinction coefficient *k* along *a*, *b* and *c* directions of (a) $LaTaON_2$, (b) $YTaON_2$, (e) $LaTiO_2N$ and (f) $YTiO_2N$. Calculated absorption coefficient α of (c) $LaTaON_2$, (d) $YTaON_2$, (g) $LaTiO_2N$ and (f) YTiO2N. The optoelectronic properties were calculated within DFT at the HSE06-level as implemented in the VASP code with a 9×9×9 k-point mesh.

Crystal structure

Atomic positions of the most stable configurations of lanthanum and yttrium oxynitrides written in a POSCAR like format:

$LaTaON_2$			
1.00			
	5.67100	0.00000	0.00000
	-0.00006	5.64274	0.00000
	0.00012	-0.02890	8.18892
Direct	*x*	*y*	*z*
La	0.99685	0.50686	0.25053
La	0.49682	0.00682	0.75050
La	0.50301	0.00676	0.25051
La	0.00335	0.50684	0.75055
Ta	0.48414	0.50813	0.49991
Ta	0.98397	0.00807	0.00047
Ta	0.51601	0.50803	0.99991
Ta	0.01588	0.00815	0.50047
O	0.30076	0.19383	0.00742
O	0.19939	0.69396	0.00732
O	0.69915	0.19356	0.50723
O	0.80080	0.69354	0.50748
N	0.79814	0.29636	0.99215
N	0.70200	0.79626	0.99204
N	0.20212	0.29599	0.49206
N	0.98167	0.99508	0.24982
N	0.48183	0.49505	0.74986
N	0.51820	0.49534	0.24986
N	0.29785	0.79600	0.49210
N	0.01808	0.99535	0.74981

YTaON$_2$			
1.00			
	5.46724	0.00000	0.00000
	-0.00933	5.63971	0.00000
	0.00602	-0.00168	7.84843
Direct	*x*	*y*	*z*
Y	0.00071	0.44985	0.24844
Y	0.50386	0.05294	0.74851
Y	0.49737	0.95017	0.24949
Y	0.99437	0.55219	0.74893
Ta	0.49124	0.51478	0.50372
Ta	0.98731	0.00764	0.99000
Ta	0.51600	0.50656	0.99859
Ta	0.99359	0.98435	0.49468
O	0.30469	0.19290	0.05220
O	0.19199	0.69265	0.05182
O	0.31418	0.19096	0.45312
O	0.81150	0.30543	0.55064
N	0.19681	0.69541	0.45281
N	0.69800	0.80234	0.54840
N	0.80325	0.30373	0.95232
N	0.69477	0.80419	0.95216
N	0.91016	0.03537	0.25241
N	0.09765	0.96837	0.75232
N	0.40265	0.46266	0.74998
N	0.58988	0.52748	0.24947

$LaTiO_2N$			
1.00			
	5.61921	0.00000	0.00000
	-0.00077	5.62651	0.00000
	-0.00140	-0.00012	7.75998
Direct	*x*	*y*	*z*
La	0.00356	0.51399	0.26794
La	0.52313	0.01402	0.76776
La	0.52296	0.00865	0.26775
La	0.00368	0.50861	0.76795
Ti	0.49232	0.51046	0.51815
Ti	0.03437	0.01105	0.01784
Ti	0.49229	0.51103	0.01786
Ti	0.03437	0.01041	0.51760
O	0.76302	0.26197	0.54919
O	0.76355	0.76200	0.48595
O	0.76357	0.26203	0.98605
O	0.76307	0.76200	0.04964
O	0.99750	0.06948	0.26773
O	0.99683	0.95385	0.76773
O	0.52965	0.56948	0.76777
O	0.52925	0.45385	0.26777
N	0.26365	0.26129	0.98914
N	0.26299	0.76130	0.04607
N	0.26312	0.26220	0.54649
N	0.26348	0.76216	0.48916

	$YTiO_2N$		
1.00			
	5.37375	0.00000	0.00000
	-0.00073	5.54449	0.00000
	-0.00002	-0.00005	7.61279
Direct	*x*	*y*	*z*
Y	0.01674	0.55687	0.25485
Y	0.51674	0.94310	0.75476
Y	0.48326	0.05678	0.25477
Y	0.98318	0.44321	0.75485
Ti	0.51991	0.49637	0.50423
Ti	0.01993	0.00351	0.00422
Ti	0.48002	0.50357	0.00428
Ti	0.98009	0.99645	0.50429
O	0.70626	0.20315	0.94280
O	0.79367	0.70320	0.94283
O	0.20629	0.29683	0.44277
O	0.89685	0.96696	0.24735
O	0.39684	0.53302	0.74735
O	0.60320	0.46700	0.24737
O	0.29379	0.79690	0.44284
O	0.10318	0.03304	0.74737
N	0.20547	0.29438	0.05079
N	0.29449	0.79436	0.05074
N	0.70556	0.20567	0.55079
N	0.79451	0.70564	0.55075

Atomic positions of the less stable configurations of lanthanum and yttrium oxynitrides written in a POSCAR like format:

$LaTaON_2$ – S1 (a in Table 1)			
1.00			
	5.69064	0.00043	0.00091
	-0.00025	5.68960	0.00006
	0.00120	0.00021	8.09561
Direct	*x*	*y*	*z*
La	-0.01437	-0.49630	0.25006
La	-0.48562	0.00366	-0.24991
La	0.48225	0.00464	0.25010
La	0.01781	-0.49537	-0.24988
Ta	-0.48649	-0.49477	-0.49937
Ta	-0.01342	0.00479	-0.00071
Ta	-0.48657	-0.49532	0.00121
Ta	-0.01334	0.00509	0.49990
O	0.28451	0.21395	-0.02633
O	0.21534	-0.28615	0.02601
O	0.28474	0.21365	-0.47382
O	0.21526	-0.28636	0.47359
N	-0.22177	0.27665	-0.47444
N	-0.27824	-0.22331	0.47423
N	-0.22202	0.27639	-0.02588
N	-0.27803	-0.22357	0.02571
N	0.02022	0.05232	0.25000
N	0.00729	-0.05119	-0.25003
N	0.47980	-0.44762	-0.25023
N	0.49268	0.44882	0.24978

$LaTaON_2$ – S2 (b in Table 1)			
1.00			
	5.70218	-0.01253	0.00090
	0.01221	5.66939	0.00316
	0.00358	0.00309	8.13720
Direct	*x*	*y*	*z*
La	-0.00438	0.48759	0.24546
La	-0.49819	0.01820	-0.25473
La	0.49945	-0.00988	0.24542
La	-0.00346	-0.48096	-0.25285
Ta	0.49584	-0.48498	0.49308
Ta	-0.01283	0.00590	-0.01115
Ta	-0.48823	-0.49756	-0.00898
Ta	-0.00295	-0.01430	0.49142
O	0.27237	0.22351	0.03275
O	0.22556	-0.27606	0.03803
O	0.29035	0.21127	0.47963
O	-0.21451	0.28240	-0.46413
N	0.22100	-0.28171	0.47304
N	-0.27661	-0.22107	-0.47262
N	-0.23027	0.27104	-0.02815
N	-0.27146	-0.22936	-0.02238
N	-0.05176	0.01782	0.25453
N	0.06013	-0.00582	-0.24581
N	0.43916	0.49209	-0.24643
N	-0.44922	0.49188	0.25386

$LaTaON_2$ – S3 (c in Table 1)			
1.00			
	5.74335	0.03894	0.01533
	-0.02829	5.70249	-0.02468
	-0.02316	-0.06524	8.02497
Direct	*x*	*y*	*z*
La	-0.00143	-0.49651	0.25222
La	-0.49620	0.00538	-0.24730
La	0.49270	0.00455	0.25245
La	-0.00574	-0.49226	-0.24959
Ta	-0.49486	0.49595	-0.48879
Ta	-0.01576	-0.00058	0.00768
Ta	0.49878	-0.48455	-0.00706
Ta	-0.00990	0.01432	0.49390
O	0.27506	0.22497	0.02884
O	-0.43863	0.48235	0.24894
O	0.26516	-0.23895	0.45840
O	0.07197	-0.01586	-0.25104
N	-0.22847	0.26392	-0.03788
N	0.23547	-0.27136	0.03613
N	-0.26348	0.23541	-0.46346
N	-0.26496	-0.23550	-0.02898
N	0.23643	0.26246	0.46990
N	-0.23590	-0.26528	-0.47368
N	-0.05964	0.00729	0.24958
N	0.43942	-0.49574	-0.25026

$LaTaON_2$ – S4 (d in Table 1)			
1.00			
	5.72486	0.15357	-0.00047
	-0.00309	5.72392	0.00000
	0.00240	0.00224	7.98496
Direct	*x*	*y*	*z*
La	0.00132	0.49809	0.25022
La	-0.49608	-0.00430	-0.24985
La	-0.49820	-0.00195	0.24979
La	0.00404	0.49460	-0.25019
Ta	-0.49012	0.48821	-0.49390
Ta	-0.00507	0.00313	0.01003
Ta	-0.48994	0.48830	-0.00605
Ta	-0.00515	0.00304	0.48981
O	0.44081	-0.44218	0.25001
O	0.24899	-0.24661	-0.44646
O	-0.04923	0.04763	-0.24998
O	0.24703	-0.24850	-0.05374
N	0.24930	0.25143	-0.00152
N	-0.24930	0.25246	0.04896
N	-0.25122	0.25057	0.45093
N	-0.25351	-0.24558	0.00139
N	0.24707	0.25370	-0.49830
N	-0.25119	-0.24786	0.49882
N	0.05182	-0.04890	0.24999
N	-0.45137	0.45472	-0.24997

$LaTaON_2$ – S5 (e in Table 1)			
1.00			
	5.72214	-0.06752	0.02509
	-0.07682	5.72738	0.01550
	-0.06507	-0.03759	7.99378
Direct	*x*	*y*	*z*
La	0.00416	-0.49655	0.25249
La	-0.49557	0.00326	-0.24753
La	-0.49701	0.00253	0.25389
La	0.00313	-0.49789	-0.24621
Ta	0.49682	0.49496	-0.48805
Ta	-0.00308	-0.00505	0.01181
Ta	-0.48710	-0.48899	-0.00398
Ta	0.01284	0.01089	0.49583
O	0.25059	0.24386	-0.05454
O	0.44786	0.44332	0.24731
O	-0.05222	-0.05659	-0.25268
O	-0.25013	-0.25518	0.44558
N	0.25114	-0.24799	0.49451
N	-0.24821	0.25270	-0.00546
N	0.24241	-0.25672	0.00108
N	-0.25635	0.24450	-0.49884
N	-0.25531	-0.24650	0.04829
N	0.24566	0.25264	-0.45176
N	0.04522	0.05138	0.24910
N	-0.45483	-0.44858	-0.25084

$YTaON_2$ – S1 (a in Table 1)			
1.00			
	5.65293	0.00002	0.00005
	-0.00009	5.45702	-0.00005
	-0.00007	0.00000	7.83394
Direct	*x*	*y*	*z*
Y	-0.04967	-0.49532	0.25003
Y	-0.45031	0.00468	-0.24999
Y	0.44757	-0.00141	0.25003
Y	0.05240	0.49859	-0.24994
Ta	-0.48441	-0.49495	-0.49954
Ta	-0.01558	0.00508	0.00043
Ta	-0.48447	-0.49498	-0.00031
Ta	-0.01555	0.00500	0.49965
O	0.30688	0.18903	-0.04856
O	0.19305	-0.31099	0.04849
O	0.30693	0.18908	-0.45149
O	0.19319	-0.31082	0.45139
N	-0.19586	0.30435	-0.45204
N	-0.30406	-0.19570	0.45198
N	-0.19596	0.30425	-0.04803
N	-0.30409	-0.19574	0.04800
N	0.03926	0.09257	0.24997
N	-0.02629	-0.09264	-0.25003
N	0.46072	-0.40743	-0.25002
N	-0.47374	0.40736	0.24998

$YTaON_2$ – S3 (c in Table 1)			
1.00			
	5.56087	0.04105	-0.00465
	0.03785	5.62722	-0.02188
	-0.00380	0.10343	7.87530
Direct	*x*	*y*	*z*
Y	-0.00486	0.46141	0.22670
Y	-0.49663	-0.03843	-0.27330
Y	0.49190	-0.04269	0.23082
Y	-0.00737	0.45921	-0.26840
Ta	0.49481	0.47933	-0.49713
Ta	-0.01397	-0.01886	0.00178
Ta	-0.49892	0.49770	-0.01500
Ta	-0.01763	-0.00631	0.49019
O	0.29193	0.22221	0.06195
O	-0.40596	-0.46843	0.25563
O	0.30819	-0.18464	0.46793
O	0.10244	0.02925	-0.24364
N	-0.20116	0.30389	-0.03285
N	0.21758	-0.27857	0.05893
N	-0.28125	0.22174	-0.44241
N	-0.29406	-0.20218	-0.03997
N	0.20705	0.30610	0.45958
N	-0.20899	-0.27540	-0.44368
N	-0.09154	0.01523	0.25180
N	0.40845	-0.48055	-0.24892

YTaON$_2$ – S4 (d in Table 1)			
1.00			
	5.57679	0.07305	-0.00021
	-0.01055	5.57699	-0.00402
	-0.01687	-0.00806	7.81755
Direct	*x*	*y*	*z*
Y	0.00836	-0.49293	0.26781
Y	-0.48943	0.00397	-0.23773
Y	0.49402	-0.00914	0.23184
Y	-0.00401	0.49051	-0.26257
Ta	-0.48981	0.48502	-0.49484
Ta	-0.00420	0.00658	0.01020
Ta	-0.48522	0.48968	-0.00544
Ta	-0.00601	0.00481	0.48995
O	0.42539	-0.42596	0.24993
O	0.29474	-0.19985	-0.43502
O	-0.06854	0.06832	-0.24996
O	0.19982	-0.29624	-0.06415
N	0.30263	0.19530	-0.00333
N	-0.20686	0.29427	0.06337
N	-0.29516	0.20685	0.43696
N	-0.30532	-0.19638	-0.00207
N	0.19526	0.30642	-0.49749
N	-0.19676	-0.30139	-0.49752
N	0.06601	-0.06517	0.25011
N	-0.43489	0.43534	-0.25006

$YTaON_2$ – S5 (e in Table 1)			
1.00			
	5.64735	-0.16586	-0.00095
	-0.00091	5.57933	-0.00160
	0.08283	-0.05706	7.82118
Direct	*x*	*y*	*z*
Y	-0.04160	-0.49635	0.22929
Y	0.45823	0.00350	-0.27066
Y	0.45660	0.00195	0.23102
Y	-0.04335	-0.49795	-0.26907
Ta	0.47761	-0.49432	-0.49507
Ta	-0.02240	0.00581	0.00503
Ta	0.49103	-0.48093	-0.00834
Ta	-0.00906	0.01910	0.49174
O	0.31415	0.19320	-0.03519
O	-0.47485	0.40433	0.25364
O	0.02514	-0.09559	-0.24635
O	-0.18611	-0.30669	0.46471
N	0.30573	-0.20915	0.46250
N	-0.19389	0.29119	-0.03748
N	0.22008	-0.29485	0.04842
N	-0.27996	0.20516	-0.45145
N	-0.28038	-0.21805	0.06288
N	0.21968	0.28178	-0.43712
N	0.03167	0.09395	0.25077
N	-0.46829	-0.40608	-0.24927

YTaON$_2$ – S6 (f in Table 1)			
1.00			
	5.52543	0.00100	-0.00003
	-0.00094	5.53759	0.04911
	0.00017	0.07385	8.05545
Direct	*x*	*y*	*z*
Y	-0.00173	0.46023	0.22730
Y	0.49831	-0.03976	-0.27269
Y	-0.49835	-0.03981	0.22728
Y	0.00161	0.46020	-0.27271
Ta	0.48664	0.49683	0.48594
Ta	-0.01333	-0.00319	-0.01407
Ta	-0.48668	0.49679	-0.01406
Ta	0.01335	-0.00320	0.48595
O	0.28891	0.21842	0.06046
O	0.21114	-0.28153	0.06048
O	-0.28884	0.21852	-0.43951
O	-0.21110	-0.28154	-0.43953
N	-0.18800	0.31351	-0.03115
N	-0.31194	-0.18653	-0.03119
N	0.18802	0.31353	0.46882
N	-0.08603	0.01096	0.25747
N	0.41395	-0.48903	-0.24254
N	-0.41400	-0.48899	0.25745
N	0.31205	-0.18643	0.46885
N	0.08602	0.01101	-0.24256

$LaTiO_2N$ – S2 (b in Table 1)			
1.00			
	5.63950	0.01941	-0.00220
	0.00373	5.59531	0.00072
	0.00342	0.00091	7.78312
Direct	*x*	*y*	*z*
La	0.02948	-0.47909	0.27717
La	-0.46765	0.00968	-0.22439
La	-0.47280	0.01337	0.27593
La	0.02320	-0.48019	-0.22326
Ti	-0.47431	0.49510	-0.47581
Ti	0.04824	0.01704	0.02618
Ti	-0.49225	-0.48245	0.02644
Ti	0.02514	0.03603	-0.47503
O	0.28192	-0.23388	0.48479
O	-0.21836	-0.23590	-0.44896
O	-0.22267	0.26213	-0.01588
O	-0.22040	-0.23731	-0.00526
O	-0.03295	0.01567	0.27242
O	0.08480	-0.00311	-0.22770
O	0.47325	-0.46677	-0.22783
O	-0.40914	-0.48756	0.27227
N	0.27708	0.26554	0.04865
N	0.27960	-0.23461	0.05581
N	0.27919	0.26619	0.49898
N	-0.22078	0.26427	-0.44474

$LaTiO_2N$ – S3 (c in Table 1)			
1.00			
	5.56405	-0.00834	-0.00615
	0.00541	5.54608	-0.00224
	0.03772	-0.08926	7.96313
Direct	*x*	*y*	*z*
La	0.00164	-0.49497	0.25053
La	-0.49518	0.00445	-0.25029
La	-0.49355	0.00141	0.25188
La	0.00824	-0.49787	-0.24771
Ti	0.49419	-0.48767	0.49116
Ti	0.01440	0.01240	-0.00691
Ti	0.49769	0.49338	0.01276
Ti	0.01048	-0.00651	-0.48784
O	-0.21341	0.29000	-0.00854
O	0.21006	-0.28647	0.00733
O	-0.28990	0.20844	-0.49390
O	-0.29109	-0.21385	-0.02168
O	0.21102	0.28340	0.47822
O	-0.21420	-0.29151	-0.48003
O	-0.03938	-0.01773	0.24813
O	0.47214	0.48228	-0.25160
N	0.28080	0.21764	0.01803
N	-0.46960	-0.48921	0.24915
N	0.28253	-0.21926	0.49221
N	0.02313	0.01166	-0.25091

$LaTiO_2N$ – S4 (d in Table 1)			
1.00			
	5.56606	-0.11647	0.00533
	0.00988	5.56669	-0.00496
	-0.05729	0.05903	7.92568
Direct	*x*	*y*	*z*
La	-0.00146	-0.49640	0.25155
La	-0.49577	0.00320	-0.24879
La	-0.49579	0.00343	0.24798
La	0.00464	0.49756	-0.25220
Ti	0.49203	-0.48991	0.49036
Ti	0.01121	-0.00816	-0.01161
Ti	0.49299	-0.48974	0.01096
Ti	0.01081	-0.00855	-0.49099
O	0.21705	0.27587	0.03157
O	-0.28590	0.21358	-0.00063
O	-0.21835	0.28094	0.49957
O	-0.22365	-0.28343	-0.03272
O	0.27568	0.22398	0.46730
O	-0.27524	-0.22503	-0.46847
O	-0.04422	-0.03148	0.25024
O	0.46895	0.45522	-0.25140
N	-0.46729	-0.47424	0.24927
N	0.22590	-0.27496	0.49945
N	0.02666	0.03193	-0.25036
N	0.27661	-0.22394	-0.00044

$LaTiO_2N$ – S5 (e in Table 1)			
1.00			
	5.56904	0.10684	0.00000
	0.00000	5.56394	0.00000
	-0.07283	-0.08505	7.94190
Direct	*x*	*y*	*z*
La	0.00542	0.49422	0.25318
La	-0.49462	-0.00588	-0.24692
La	-0.49113	-0.00245	0.24965
La	0.00875	0.49745	-0.25039
Ti	-0.48339	-0.49058	0.49238
Ti	0.01655	0.00946	-0.00734
Ti	0.49608	0.48908	0.01275
Ti	-0.00370	-0.01088	-0.48706
O	0.27663	-0.21901	0.46721
O	-0.22327	0.28110	-0.03282
O	0.21592	-0.27967	0.03008
O	-0.28374	0.22062	-0.46988
O	-0.28796	-0.21633	-0.00229
O	0.21218	0.28354	0.49774
O	-0.03896	0.03433	0.24793
O	0.46082	-0.46557	-0.25198
N	0.27752	0.21984	0.00015
N	-0.47019	0.47027	0.24872
N	0.02991	-0.02969	-0.25129
N	-0.22283	-0.27983	-0.49984

$LaTiO_2N$ – S6 (f in Table 1)			
1.00			
	5.65552	-0.00153	-0.00023
	0.00027	5.57646	-0.00039
	-0.00018	-0.00001	7.79790
Direct	*x*	*y*	*z*
La	0.00598	-0.46811	0.26652
La	-0.49391	0.03174	-0.23346
La	0.49887	0.03180	0.26656
La	-0.00111	-0.46843	-0.23351
Ti	-0.47707	-0.46797	-0.48534
Ti	0.02298	0.03176	0.01446
Ti	0.48199	-0.46821	0.01458
Ti	-0.01798	0.03198	-0.48557
O	-0.24740	0.28157	-0.02516
O	-0.24772	-0.21844	-0.02563
O	0.25204	0.28161	0.47446
O	-0.05927	0.03067	0.25862
O	0.44076	-0.46917	-0.24134
O	-0.43584	-0.46799	0.25865
O	0.25275	-0.21843	0.47482
O	0.06417	0.03203	-0.24137
N	0.25253	0.28138	0.04047
N	0.25235	-0.21863	0.03986
N	-0.24791	0.28099	-0.46041
N	-0.24731	-0.21891	-0.45946

$YTiO_2N$ – S1 (a in Table 1)			
1.00			
	5.57303	-0.00017	0.00008
	-0.00006	5.35507	-0.00005
	0.00005	-0.00013	7.59911
Direct	*x*	*y*	*z*
Y	-0.06420	-0.48894	0.24642
Y	-0.44150	0.01101	-0.25359
Y	0.44427	-0.02187	0.24640
Y	0.05003	0.47810	-0.25358
Ti	0.47862	0.48363	0.49723
Ti	0.01566	-0.01637	-0.00280
Ti	0.47857	0.48356	-0.00435
Ti	0.01571	-0.01633	0.49561
O	-0.20809	0.29575	-0.44870
O	-0.29752	-0.20419	0.44150
O	-0.20811	0.29577	-0.05851
O	-0.29752	-0.20419	0.05129
O	0.02558	0.09807	0.24640
O	-0.04099	-0.10616	-0.25360
O	0.46880	-0.40198	-0.25359
O	-0.46466	0.39381	0.24641
N	0.29355	0.20171	-0.05512
N	0.20075	-0.29831	0.04792
N	0.29354	0.20173	-0.45206
N	0.20080	-0.29829	0.44487

$YTiO_2N$ – S2 (b in Table 1)			
1.00			
	5.36528	-0.00436	0.00095
	0.00149	5.55949	-0.00142
	-0.00555	-0.00732	7.60519
Direct	*x*	*y*	*z*
Y	0.01069	0.44107	0.24767
Y	-0.48371	0.05227	-0.24938
Y	0.48359	-0.06242	0.25146
Y	-0.02192	-0.44343	-0.25235
Ti	-0.49226	0.47869	0.49653
Ti	0.01844	-0.00752	0.00278
Ti	0.47643	0.49292	-0.00091
Ti	0.00964	0.01499	0.49820
O	0.19244	-0.29834	0.44204
O	-0.30695	-0.20694	-0.44828
O	-0.20622	0.29665	-0.06020
O	-0.29477	-0.20634	-0.06030
O	-0.10725	0.02990	0.24417
O	0.09760	-0.03685	-0.25492
O	0.39489	0.46824	-0.25318
O	-0.39996	-0.46538	0.24659
N	0.29508	0.20139	0.04881
N	0.20358	-0.29668	0.04771
N	0.28762	0.20193	0.44601
N	-0.21301	0.29231	-0.45275

$YTiO_2N$ – S3 (c in Table 1)			
1.00			
	5.43188	-0.06525	0.00131
	0.00132	5.44801	0.00231
	-0.00460	0.04617	7.79253
Direct	*x*	*y*	*z*
Y	0.00282	0.45104	0.22624
Y	0.49923	-0.04673	-0.27148
Y	-0.49962	-0.04040	0.22218
Y	0.00355	0.45899	-0.27887
Ti	-0.49918	0.49320	0.47571
Ti	0.00762	-0.00809	-0.02324
Ti	0.49072	0.47494	-0.00298
Ti	0.01426	-0.02445	0.49290
O	-0.19973	0.31044	-0.04428
O	0.20263	-0.28760	0.04875
O	-0.30078	0.21667	-0.44656
O	-0.31282	-0.18607	-0.03302
O	0.18797	0.30141	0.46469
O	-0.22070	-0.29071	-0.45211
O	-0.09563	0.02286	0.25175
O	0.40944	-0.47814	-0.24746
N	0.28278	0.21242	0.03874
N	-0.41957	-0.49827	0.24740
N	0.28900	-0.20614	0.45756
N	0.07357	0.00045	-0.25392

$YTiO_2N$ – S4 (d in Table 1)			
1.00			
	5.41221	-0.10236	0.00511
	-0.01783	5.41412	0.00519
	-0.04166	-0.04251	7.74429
Direct	*x*	*y*	*z*
Y	-0.00885	0.48531	0.26026
Y	0.49787	-0.01302	-0.24479
Y	-0.48503	0.00954	0.24031
Y	0.01385	-0.49727	-0.25476
Ti	0.49422	-0.49224	0.48916
Ti	0.01345	-0.01885	-0.00649
Ti	0.49337	-0.49470	0.01112
Ti	0.01806	-0.01313	-0.49283
O	0.31574	0.18763	-0.00193
O	-0.19665	0.31339	-0.04646
O	-0.31365	0.19514	-0.45469
O	-0.31401	-0.18299	-0.00069
O	0.18334	0.31355	-0.49906
O	-0.18741	-0.31626	-0.49808
O	-0.05963	0.06013	0.24980
O	0.44663	-0.44614	-0.25015
N	-0.45261	0.45277	0.24988
N	0.30361	-0.19405	0.45559
N	0.04453	-0.04475	-0.25006
N	0.19319	-0.30405	0.04386

$YTiO_2N$ – S5 (e in Table 1)			
1.00			
	5.43088	0.05351	0.00409
	-0.01831	5.43104	0.00380
	-0.02322	-0.02229	7.70372
Direct	*x*	*y*	*z*
Y	-0.00280	0.48333	0.26112
Y	0.49705	-0.01659	-0.23887
Y	-0.48204	0.00421	0.24023
Y	0.01819	-0.49586	-0.25972
Ti	-0.48527	-0.49610	0.49125
Ti	0.01465	0.00386	-0.00889
Ti	0.49660	0.48578	0.00933
Ti	-0.00351	-0.01432	-0.49084
O	0.29873	-0.19437	0.44527
O	-0.20088	0.30614	-0.05438
O	0.19216	-0.30083	0.05258
O	-0.30807	0.19882	-0.44759
O	-0.31332	-0.18686	0.00043
O	0.18670	0.31281	-0.49949
O	-0.06271	0.06360	0.24985
O	0.43734	-0.43631	-0.25019
N	0.30409	0.19574	0.00003
N	-0.44551	0.44573	0.24988
N	0.05447	-0.05431	-0.25015
N	-0.19590	-0.30449	-0.49986

Thermodynamic data used to compute the stability of the phases:

Compound	$\Delta_f H°$ / kJ.mol^{-1}
La_2O_3	-1793.3
Y_2O_3	-1933.0
TiO_2	-940.0
Ta_3N_5	-849.7