

**Table S1** Experimental ( $d_{hkl}^{exp}$ ) and refined ( $d_{hkl}^{cal}$ ) lattice spacings of SrTiO<sub>3</sub> and relative deviation. The experimental datasets are based on measurements of angles  $\omega$  (1) and angles  $2\theta$  (2).

Bragg Reflection			Evaluation using (1) (a = 3.905185 Å)			Evaluation using (2) (a = 3.905350 Å)		
h	k	l	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$
0	0	1	3.90513	3.90519	$1.41 \times 10^{-5}$	3.90558	3.90535	$6.40 \times 10^{-5}$
0	0	2	1.95250	1.95259	$4.74 \times 10^{-5}$	1.95269	1.95268	$1.28 \times 10^{-5}$
0	0	3	1.30175	1.30173	$1.67 \times 10^{-5}$	1.30179	1.30178	$1.28 \times 10^{-5}$
0	0	4	0.97634	0.97630	$4.48 \times 10^{-5}$	0.97634	0.97634	$2.56 \times 10^{-6}$

**Table S2** Experimental ( $d_{hkl}^{exp}$ ) and refined ( $d_{hkl}^{cal}$ ) lattice spacings of DyScO<sub>3</sub> and relative deviation. The experimental datasets are based on measurements of angles  $\omega$  (1) and angles  $2\theta$  (2).

Bragg Reflection			Evaluation using (1) (a = 5.442441 Å, b = 5.719317 Å, c = 7.904240 Å)			Evaluation using (2) (a = 5.442393 Å, b = 5.719398 Å, c = 7.904408 Å)		
h	k	l	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$
0	0	2	3.95165	3.95212	$1.19 \times 10^{-4}$	3.95230	3.95220	$2.35 \times 10^{-5}$
1	1	0	3.94242	3.94264	$5.48 \times 10^{-5}$	3.94261	3.94264	$8.81 \times 10^{-6}$
0	0	4	1.97602	1.97606	$1.82 \times 10^{-5}$	1.97604	1.97610	$3.24 \times 10^{-5}$
2	2	0	1.97126	1.97132	$2.95 \times 10^{-5}$	1.97134	1.97132	$8.95 \times 10^{-6}$
2	2	1	1.91277	1.91273	$2.13 \times 10^{-5}$	1.91267	1.91273	$3.42 \times 10^{-5}$
2	3	0	1.56134	1.56139	$3.09 \times 10^{-5}$	1.56143	1.56140	$2.00 \times 10^{-5}$
3	2	0	1.53185	1.53189	$2.73 \times 10^{-5}$	1.53189	1.53189	$9.81 \times 10^{-7}$
0	0	6	1.31737	1.31737	$1.90 \times 10^{-10}$	1.31740	1.31740	$2.15 \times 10^{-6}$
3	3	0	1.31419	1.31421	$1.68 \times 10^{-5}$	1.31418	1.31421	$2.66 \times 10^{-5}$
3	3	1	1.29642	1.29642	$4.02 \times 10^{-6}$	1.29641	1.29642	$6.36 \times 10^{-6}$
2	4	0	1.26577	1.26574	$2.36 \times 10^{-5}$	1.26576	1.26575	$6.39 \times 10^{-6}$
3	3	2	1.24707	1.24707	$1.67 \times 10^{-8}$	1.24707	1.24708	$4.04 \times 10^{-6}$
4	2	0	1.22863	1.22863	$7.89 \times 10^{-11}$	1.22864	1.22862	$1.27 \times 10^{-5}$
2	4	2	1.20542	1.20543	$6.18 \times 10^{-6}$	1.20544	1.20544	$1.35 \times 10^{-8}$
4	2	2	1.17325	1.17324	$5.97 \times 10^{-6}$	1.17320	1.17324	$3.44 \times 10^{-5}$
3	4	0	1.12297	1.12297	$1.73 \times 10^{-6}$	1.12298	1.12297	$5.21 \times 10^{-6}$
4	3	0	1.10748	1.10748	$4.52 \times 10^{-6}$	1.10750	1.10748	$1.46 \times 10^{-5}$
5	2	0	1.01729	1.01729	$3.92 \times 10^{-6}$	1.01728	1.01728	$1.12 \times 10^{-9}$
0	0	8	0.98805	0.98803	$1.75 \times 10^{-5}$	0.98805	0.98805	$2.21 \times 10^{-9}$
4	4	0	0.98567	0.98566	$1.11 \times 10^{-5}$	0.98565	0.98566	$1.13 \times 10^{-5}$
4	4	2	0.95637	0.95636	$5.66 \times 10^{-6}$	0.95637	0.95637	$2.39 \times 10^{-6}$
0	6	0	0.95326	0.95322	$4.26 \times 10^{-5}$	0.95325	0.95323	$1.78 \times 10^{-5}$
6	0	0	0.90708	0.90707	$7.13 \times 10^{-6}$	0.90706	0.90707	$6.08 \times 10^{-6}$
4	4	4	0.88202	0.88202	$3.59 \times 10^{-6}$	0.88201	0.88203	$2.09 \times 10^{-5}$

**Table S3** Experimental ( $d_{hkl}^{exp}$ ) and refined ( $d_{hkl}^{cal}$ ) lattice spacings of NdGaO<sub>3</sub> and relative deviation. The experimental datasets are based on measurements of angles  $\omega$  (1) and angles  $2\theta$  (2).

Bragg Reflection			Evaluation using (1) (a = 5.428440 Å, b = 5.498356 Å, c = 7.708831 Å)			Evaluation using (2) (a = 5.428380 Å, b = 5.498458 Å, c = 7.708924 Å)		
h	k	l	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$	$d_{hkl}^{exp}$ (Å)	$d_{hkl}^{cal}$ (Å)	$ d_{hkl}^{exp} - d_{hkl}^{cal} /d_{hkl}^{exp}$
0	0	2	3.85628	3.85442	$4.83 \times 10^{-4}$	3.85618	3.85446	$4.45 \times 10^{-4}$
2	2	0	1.93137	1.93148	$5.92 \times 10^{-5}$	1.93148	1.93149	$5.73 \times 10^{-6}$
0	0	4	1.92732	1.92721	$5.69 \times 10^{-5}$	1.92742	1.92723	$9.98 \times 10^{-5}$
2	2	1	1.87351	1.87357	$3.21 \times 10^{-5}$	1.87349	1.87358	$4.68 \times 10^{-5}$
3	2	0	1.51146	1.51147	$3.93 \times 10^{-6}$	1.51140	1.51146	$4.15 \times 10^{-5}$
2	3	0	1.51890	1.51892	$1.55 \times 10^{-5}$	1.51894	1.51894	$1.68 \times 10^{-6}$
3	3	0	1.28764	1.28765	$1.26 \times 10^{-5}$	1.28767	1.28766	$7.21 \times 10^{-6}$
0	0	6	1.28481	1.28481	$2.62 \times 10^{-9}$	1.28482	1.28482	$1.31 \times 10^{-9}$
3	3	1	1.27006	1.27006	$2.42 \times 10^{-9}$	1.27004	1.27007	$1.95 \times 10^{-5}$
2	4	0	1.22631	1.22630	$1.24 \times 10^{-5}$	1.22631	1.22631	$1.16 \times 10^{-8}$
4	2	0	1.21699	1.21692	$6.15 \times 10^{-5}$	1.21698	1.21691	$5.86 \times 10^{-5}$
2	4	2	1.16862	1.16858	$3.63 \times 10^{-5}$	1.16857	1.16859	$1.88 \times 10^{-5}$
3	4	0	1.09460	1.09458	$2.26 \times 10^{-5}$	1.09460	1.09459	$1.49 \times 10^{-5}$
4	3	0	1.09065	1.09066	$9.45 \times 10^{-6}$	1.09063	1.09066	$2.72 \times 10^{-5}$
4	4	0	0.96576	0.96574	$1.85 \times 10^{-5}$	0.96576	0.96575	$1.50 \times 10^{-5}$
0	0	8	0.96358	0.96360	$1.92 \times 10^{-5}$	0.96359	0.963616	$2.22 \times 10^{-5}$
4	4	2	0.93680	0.93679	$1.59 \times 10^{-5}$	0.93679	0.93679	$1.22 \times 10^{-6}$
0	6	0	0.91643	0.91639	$4.07 \times 10^{-5}$	0.91643	0.91641	$2.23 \times 10^{-5}$
6	0	0	0.90474	0.90474	$1.79 \times 10^{-8}$	0.90473	0.90473	$9.92 \times 10^{-9}$