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

Supporting Information

New insights into the luminescent properties of Na stabilized Ga – Ti oxides homologous series

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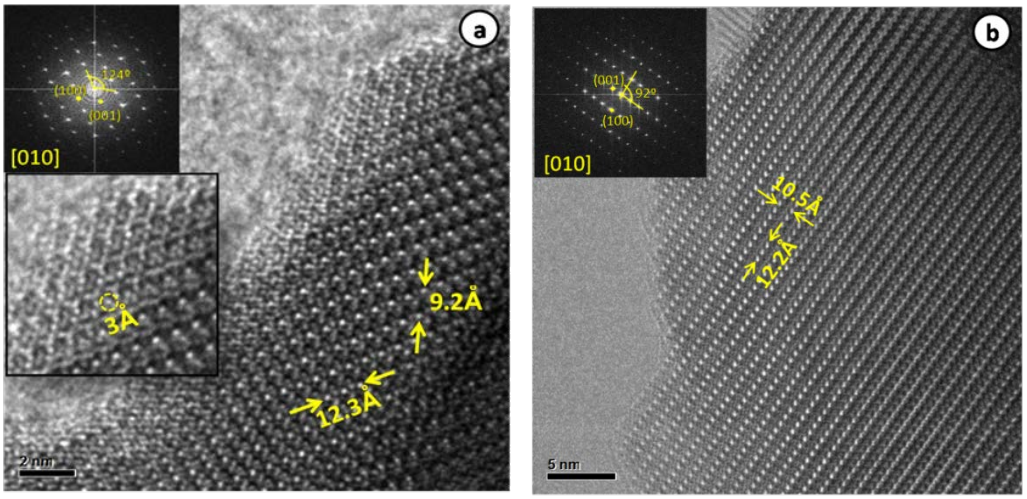
- HRTEM study of NGT1, NGT2 and NGT3 samples

Figure ES1(a) shows a representative image of NGT1 sample along the [010] zone axis. The corresponding Fourier Transform can be understood on the basis of a monoclinic unit cell with $\beta \approx 124^0$. In the image, a highly ordered and crystalline material is observed, where the size and shape of the hexagonal tunnels are visualized. Additionally, HRTEM micrographs along [010] and [001] zone axes for NGT2 and NGT3 are shown (Figure ES1(b) and (c)) for an exhaustive study of these phases. Cell parameters of all oxides are indicated in each image. This information has been crucial in order to confirm the structure of these materials, which is in good agreement with the XRD information.



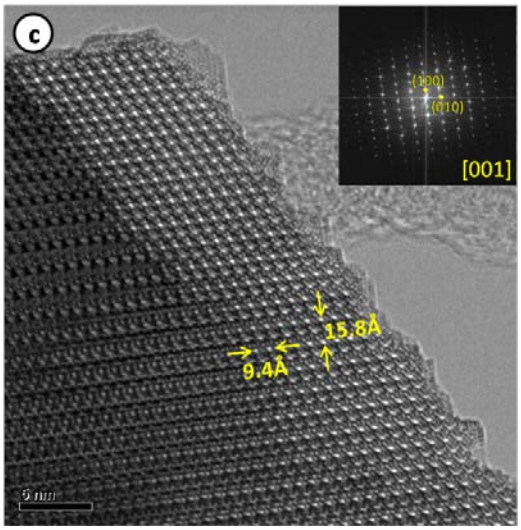


Figure S1. (a) Representative HRTEM image of NGT1 along the [010] zone axis. The upper inset shows the corresponding FT where β angle is measured. The inset below shows an enhancement of a thin area of the crystal at higher magnification where the size and shape of the hexagonal channel is clearly visible with an average diameter of 3 Å. (b) HRTEM image of NGT2 along [010] zone axis. The insets show the corresponding FT where β angle is measured (c) HRTEM image of NGT3 along [001]. The inset shows the corresponding FT. Cell parameters are indicated in each image.

- DFT calculations

Atomic coordinates of the three terms studied in this work used in the DFT calculations.

Table ES1.

$Na_{0.6}Ga_{4.6\pm0.1}Ti_{0.3}O_8$

90 atoms	x (Å)	y (Å)	z (Å)
Ga	6,16170	-0,03631	-0,00032
Ti	1,13970	-0,03617	7,90318
Ga	6,16062	3,02690	0,00004
Ti	6,16080	-2,98812	0,00021
Ti	-0,00009	-1,49763	-0,00001
Ti	-5,02209	-1,49750	7,90349
Ti	12,32214	-1,49757	-0,00001
Ti	7,30013	-1,49744	7,90349
Ga	0,00013	1,53671	-0,00004
Ga	-5,02188	1,53685	7,90346
Ga	0,00018	4,48792	-0,00005
Ga	-5,02183	4,48806	7,90345
Ga	1,37263	0,00487	2,81317
Ga	1,35919	3,02124	2,77871
Ga	1,37776	-3,02477	2,83867
Ga	5,92753	0,00507	5,09034
Ga	5,94093	3,02134	5,12454

Ga	5,92235	-3,02471	5,06484
Ga	7,52074	-1,50311	2,77942
Ga	7,53866	1,49970	2,83844
Ga	7,53345	-4,51941	2,81302
Ga	-0,22015	-1,50327	5,12475
Ga	-0,23857	1,49967	5,06475
Ga	-0,23348	-4,51942	5,09026
Ga	10,51015	-0,01959	2,37796
Ga	10,52326	3,03732	2,35944
Ga	10,56154	-3,01251	2,42796
Ga	-3,20975	-0,01975	5,52548
Ga	-3,22303	3,03718	5,54396
Ga	-3,26126	-3,01273	5,47562
Ga	4,36270	-1,48717	2,35937
Ga	4,40029	1,51195	2,42792
Ga	4,34875	4,50485	2,37835
Ga	2,93808	-1,48734	5,54411
Ga	2,89977	1,51198	5,47559
Ga	2,95121	4,50479	5,52562
O	-0,49215	-0,00333	3,67171
O	-0,49934	3,01829	3,68460
O	-0,45597	-3,00867	3,70930
O	7,79252	-0,00318	4,23170
O	7,79985	3,01819	4,21860
O	7,75638	-3,00927	4,19419
O	5,66178	-1,50648	3,68498
O	5,70497	1,51570	3,70914
O	5,66898	4,52124	3,67196
O	1,63876	-1,50630	4,21870
O	1,59522	1,51580	4,19420
O	1,63138	4,52139	4,23173
O	0,15855	0,01734	6,19837
O	0,15450	3,01164	6,21017
O	0,09363	-3,02686	6,23650
O	7,14109	0,01703	1,70520
O	7,14549	3,01159	1,69325
O	7,20607	-3,02662	1,66719
O	6,31578	-1,51288	6,21022
O	6,25520	1,49767	6,23634
O	6,31986	-4,50708	6,19830
O	0,98475	-1,51301	1,69320
O	1,04530	1,49748	1,66701
O	0,98067	-4,50713	1,70505
O	-3,90047	-0,01261	7,22935
O	-3,88085	2,99582	7,24086

O	-3,91657	-2,97742	7,20177
O	11,20086	-0,01256	0,67404
O	11,18134	2,99584	0,66258
O	11,21691	-2,97731	0,70170
O	2,28004	-1,52891	7,24095
O	2,24436	1,54714	7,20185
O	2,26043	4,51200	7,22948
O	5,01989	-1,52853	0,66223
O	5,05549	1,54721	0,70166
O	5,03948	4,51187	0,67429
O	3,32636	0,02270	2,49121
O	3,31936	2,99677	2,50437
O	3,31789	-3,01524	2,43675
O	3,97391	0,02280	5,41296
O	3,98078	2,99676	5,39972
O	3,98254	-3,01551	5,46717
O	9,48065	-1,52762	2,50411
O	9,47873	1,50912	2,43632
O	9,48730	-4,50164	2,49059
O	-2,18038	-1,52783	5,39921
O	-2,17853	1,50902	5,46695
O	-2,18716	-4,50186	5,41225
Na	3,27315	-3,03943	-0,03319
Na	-1,74886	-3,03929	7,87031
Na	9,04851	-3,04099	0,03375
Na	9,43468	1,48447	-0,03361
Na	4,41267	1,48461	7,86989
Na	2,88776	1,48334	0,03295

$Na_{0.7}Ga_{4.7}Ti_{1.2}O_{10}$

103 atoms	x (Å)	y (Å)	z (Å)
Na	0,324920	0,009609	-5,098970
Na	0,275795	3,008707	-5,159145
Na	0,237023	-3,042835	-5,202367
Na	-5,869352	2,141083	-5,160120
Na	6,197664	2,144736	-5,160120
Na	6,192499	-2,108883	-5,169714
Na	-5,874518	-2,112536	-5,169714
Ga	1,098363	-0,000741	-8,710766
Ga	1,101690	3,013232	-8,706003
Ga	1,110377	-3,027705	-8,721049
Ga	-0,693686	0,002367	-1,676059
Ga	-0,700067	3,014571	-1,693705
Ga	-0,710011	-3,023438	-1,686640

Ga	-4,935067	-1,518137	-8,680576
Ga	-4,926203	1,507458	-8,684026
Ga	-4,936210	-4,532078	-8,673056
Ga	5,305493	-1,511173	-1,723235
Ga	5,296934	1,513816	-1,724091
Ga	5,315990	-4,528608	-1,735950
Ga	4,262779	0,002637	-9,358184
Ga	4,249638	3,028306	-9,332197
Ga	4,250547	-3,040387	-9,340321
Ga	-3,896100	0,002993	-1,020181
Ga	-3,875147	3,039918	-1,065961
Ga	-3,875429	-3,049329	-1,060744
Ga	-1,754983	-1,518061	-9,391424
Ga	-1,772081	1,529578	-9,354510
Ga	-1,771386	4,507471	-9,351989
Ga	2,169569	-1,495108	-1,051315
Ga	2,188750	1,515240	-1,085474
Ga	2,172108	4,511127	-1,057926
Ga	3,357208	0,015997	-3,873315
Ga	3,319124	3,002961	-3,899397
Ti	3,264002	-3,047111	-3,909771
Ti	-2,874837	0,025171	-6,506215
Ga	-2,931589	3,034635	-6,520185
Ti	-2,880984	-3,050843	-6,512240
Ti	-2,704612	-1,531238	-3,883567
Ti	-2,687391	1,520897	-3,892860
Ga	-2,656307	4,521658	-3,894099
Ti	3,086363	-1,514832	-6,486170
Ti	3,090157	1,532523	-6,463174
Ga	3,058108	4,524245	-6,520421
O	2,376518	0,002999	-10,065226
O	2,368529	3,005790	-10,077298
O	2,369479	-3,021101	-10,098024
O	-1,990766	0,008500	-0,326102
O	-1,988328	3,006528	-0,333211
O	-1,990027	-3,019446	-0,318370
O	-3,666164	-1,525093	-10,063343
O	-3,677087	1,501535	-10,085923
O	-3,676566	-4,522098	-10,071809
O	4,071044	-1,528555	-0,317225
O	4,078686	1,519531	-0,299974
O	4,074600	-4,518878	-0,331007
O	1,787956	-0,005991	-7,009891
O	1,789590	2,991830	-7,009798

O	1,803815	-3,004353	-7,028323
O	-1,401912	0,001075	-3,378008
O	-1,398601	2,970289	-3,397336
O	-1,411240	-2,980357	-3,387354
O	-4,158255	-1,533402	-7,002461
O	-4,162284	1,477544	-7,004985
O	-4,118113	-4,487943	-7,032196
O	4,567442	-1,545822	-3,403029
O	4,586739	1,520197	-3,406750
O	4,514824	-4,489382	-3,377416
O	2,563928	-0,007409	-2,162032
O	2,534755	3,024720	-2,182183
O	2,505846	-3,017415	-2,205990
O	-2,167608	-0,014395	-8,219667
O	-2,159162	3,016519	-8,228432
O	-2,119943	-3,012229	-8,202917
O	-3,461714	-1,501676	-2,190602
O	-3,468430	1,497428	-2,209615
O	-3,433992	4,527957	-2,184679
O	3,855634	-1,507198	-8,206507
O	3,864126	1,500394	-8,191359
O	3,840347	4,529129	-8,231182
O	4,081956	-0,018079	-5,795864
O	4,071879	2,977452	-5,759614
O	4,083478	-2,953352	-5,776738
O	-3,671120	-0,010101	-4,617458
O	-3,657026	2,950400	-4,668915
O	-3,692482	-2,938162	-4,628433
O	-1,846875	-1,501228	-5,784055
O	-1,831643	1,428541	-5,779277
O	-1,856599	-4,486393	-5,727498
O	2,227648	-1,538909	-4,639930
O	2,231757	1,478581	-4,662643
O	2,244606	-4,492849	-4,677579
O	6,145429	-0,001563	-8,893057
O	6,142838	3,020800	-8,872279
O	6,135137	-3,019562	-8,883174
O	-5,751204	-0,002731	-1,503363
O	-5,743235	3,017218	-1,518627
O	-5,739353	-3,019641	-1,512969
O	0,100858	-1,512912	-8,934608
O	0,093028	1,502430	-8,928049
O	0,102766	4,528041	-8,935872
O	0,277033	-1,512558	-1,453624

O	0,285924	1,507596	-1,452713
O	0,277779	4,530632	-1,485519

$Na_{0.8}Ga_{4.8}Ti_{2.1}O_{12}$

137 atoms	x (Å)	y (Å)	z (Å)
Na	0,00000	0,00000	0,51428
Na	0,00000	0,00000	3,50428
Na	0,00000	0,00000	-2,47572
Na	-7,91000	4,66500	-0,51428
Na	-7,91000	-4,66500	-0,51428
Na	7,91000	4,66500	-0,51428
Na	7,91000	-4,66500	-0,51428
Na	-7,91000	4,66500	2,47572
Na	-7,91000	-4,66500	2,47572
Na	7,91000	4,66500	2,47572
Na	7,91000	-4,66500	2,47572
Ti	2,28283	2,79060	0,00000
Ti	2,28283	2,79060	2,99000
Ga	2,28283	2,79060	-2,99000
Ti	-2,28283	-2,79060	0,00000
Ti	-2,28283	-2,79060	2,99000
Ga	-2,28283	-2,79060	-2,99000
Ti	5,62717	-1,87440	0,00000
Ti	5,62717	-1,87440	2,99000
Ga	5,62717	-1,87440	-2,99000
Ti	-5,62717	1,87440	0,00000
Ti	-5,62717	1,87440	2,99000
Ga	-5,62717	1,87440	-2,99000
Ga	3,15609	0,02053	-1,49500
Ga	3,15609	0,02053	1,49500
Ti	3,15609	0,02053	4,48500
Ga	-3,15609	-0,02053	-1,49500
Ga	-3,15609	-0,02053	1,49500
Ti	-3,15609	-0,02053	4,48500
Ga	4,75391	-4,64447	-1,49500
Ga	4,75391	4,68553	-1,49500
Ga	4,75391	-4,64447	1,49500
Ga	4,75391	4,68553	1,49500
Ti	4,75391	-4,64447	4,48500
Ti	4,75391	4,68553	4,48500
Ga	-4,75391	4,64447	-1,49500
Ga	-4,75391	-4,68553	-1,49500
Ga	-4,75391	4,64447	1,49500
Ga	-4,75391	-4,68553	1,49500

Ti	-4,75391	4,64447	4,48500
Ti	-4,75391	-4,68553	4,48500
Ga	5,58288	2,06006	0,00000
Ga	5,58288	2,06006	2,99000
Ga	5,58288	2,06006	-2,99000
Ga	-5,58288	-2,06006	0,00000
Ga	-5,58288	-2,06006	2,99000
Ga	-5,58288	-2,06006	-2,99000
Ga	2,32712	-2,60494	0,00000
Ga	2,32712	-2,60494	2,99000
Ga	2,32712	-2,60494	-2,99000
Ga	-2,32712	2,60494	0,00000
Ga	-2,32712	2,60494	2,99000
Ga	-2,32712	2,60494	-2,99000
Ga	0,00000	4,66500	-1,49500
Ga	0,00000	-4,66500	-1,49500
Ga	0,00000	4,66500	1,49500
Ga	0,00000	-4,66500	1,49500
Ga	0,00000	4,66500	4,48500
Ga	0,00000	-4,66500	4,48500
Ga	-7,91000	0,00000	-1,49500
Ga	7,91000	0,00000	-1,49500
Ga	-7,91000	0,00000	1,49500
Ga	7,91000	0,00000	1,49500
Ti	-7,91000	0,00000	4,48500
Ti	7,91000	0,00000	4,48500
O	2,27808	0,95166	0,00000
O	2,27808	0,95166	2,99000
O	2,27808	0,95166	-2,99000
O	-2,27808	-0,95166	0,00000
O	-2,27808	-0,95166	2,99000
O	-2,27808	-0,95166	-2,99000
O	5,63192	-3,71334	0,00000
O	5,63192	-3,71334	2,99000
O	5,63192	-3,71334	-2,99000
O	-5,63192	3,71334	0,00000
O	-5,63192	3,71334	2,99000
O	-5,63192	3,71334	-2,99000
O	4,66690	1,19424	-1,49500
O	4,66690	1,19424	1,49500
O	4,66690	1,19424	4,48500
O	-4,66690	-1,19424	-1,49500
O	-4,66690	-1,19424	1,49500
O	-4,66690	-1,19424	4,48500

O	3,24310	-3,47076	-1,49500
O	3,24310	-3,47076	1,49500
O	3,24310	-3,47076	4,48500
O	-3,24310	3,47076	-1,49500
O	-3,24310	3,47076	1,49500
O	-3,24310	3,47076	4,48500
O	7,02408	0,97032	0,00000
O	7,02408	0,97032	2,99000
O	7,02408	0,97032	-2,99000
O	-7,02408	-0,97032	0,00000
O	-7,02408	-0,97032	2,99000
O	-7,02408	-0,97032	-2,99000
O	0,88592	-3,69468	0,00000
O	0,88592	-3,69468	2,99000
O	0,88592	-3,69468	-2,99000
O	-0,88592	3,69468	0,00000
O	-0,88592	3,69468	2,99000
O	-0,88592	3,69468	-2,99000
O	1,45544	3,35880	-1,49500
O	1,45544	3,35880	1,49500
O	1,45544	3,35880	4,48500
O	-1,45544	-3,35880	-1,49500
O	-1,45544	-3,35880	1,49500
O	-1,45544	-3,35880	4,48500
O	6,45456	-1,30620	-1,49500
O	6,45456	-1,30620	1,49500
O	6,45456	-1,30620	4,48500
O	-6,45456	1,30620	1,49500
O	-6,45456	1,30620	4,48500
O	3,95500	3,55473	0,00000
O	3,95500	3,55473	2,99000
O	3,95500	3,55473	-2,99000
O	-3,95500	-3,55473	0,00000
O	-3,95500	-3,55473	2,99000
O	-3,95500	-3,55473	-2,99000
O	3,95500	-1,11027	0,00000
O	3,95500	-1,11027	2,99000
O	3,95500	-1,11027	-2,99000
O	-3,95500	1,11027	0,00000
O	-3,95500	1,11027	2,99000
O	-3,95500	1,11027	-2,99000
O	6,10652	3,20019	-1,49500
O	6,10652	3,20019	1,49500
O	6,10652	3,20019	4,48500

O	-6,10652	-3,20019	-1,49500
O	-6,10652	-3,20019	1,49500
O	-6,10652	-3,20019	4,48500
O	1,80348	-1,46481	-1,49500
O	1,80348	-1,46481	1,49500
O	1,80348	-1,46481	4,48500
O	-1,80348	1,46481	-1,49500
O	-1,80348	1,46481	1,49500
O	-1,80348	1,46481	4,48500