Disorder in $La_{1-x}Ba_{1+x}GaO_{4-x/2}$ ionic conductor: resolving Pair Distribution Function through insight from first principles modelling

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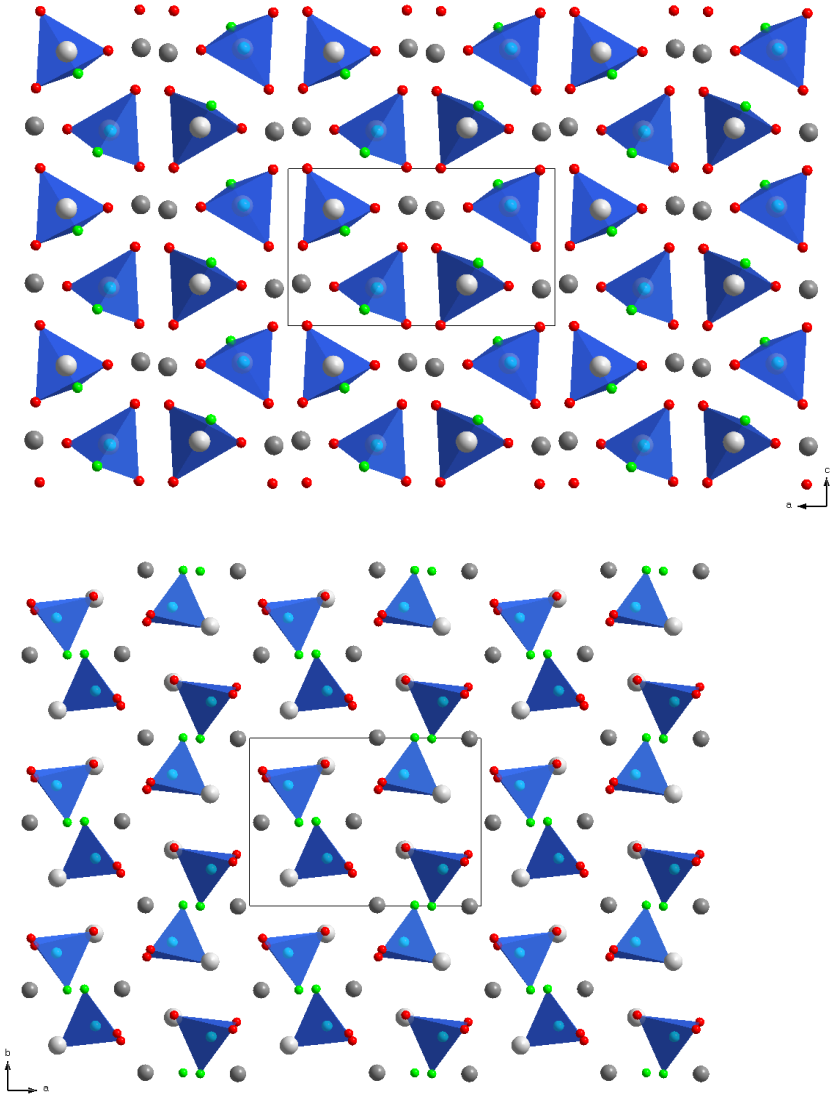

Figure SI1. View of tetrahedral connectivity in $LaBaGaO_4$ along *b* (top) and *c* axis (bottom).

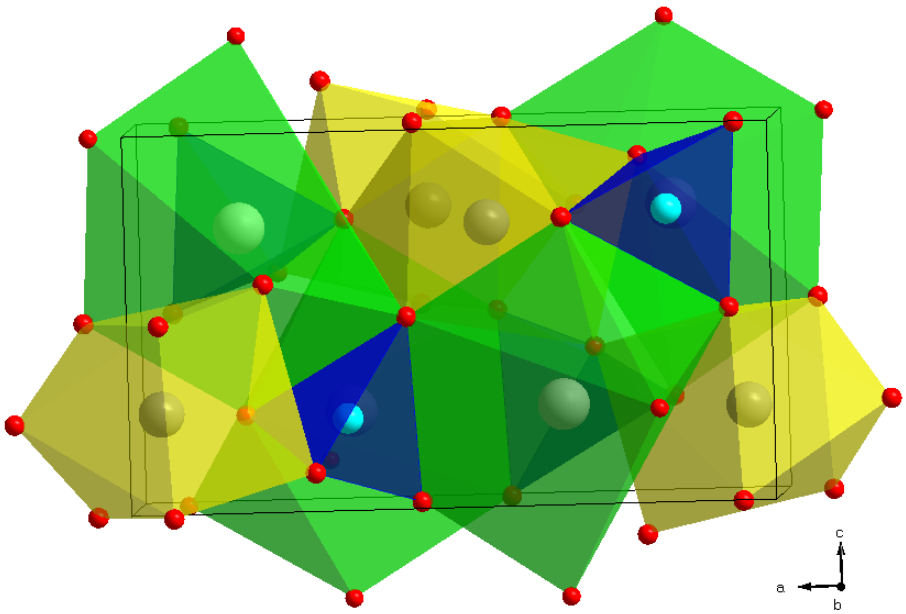

Figure SI2. Unit cell of $LaBaGaO_4$ highlighting the polyhedra characteristic of Ga (blue), Ba (green) and La (yellow).

Table SI1. Interatomic distances of interest (Å) from DFT.

	LaBaGaO4	model 1	model 2	model 3	model 4
Ga_A - O br	-	2.114	2.071	2.036	1.994
Ga_A - O	1.846	1.765	1.809	1.806	1.771
	1.864	1.852	1.755	1.870	1.882
	1.842	1.821	1.805	1.786	1.794
	1.838	-	-	-	-
Ga_B - O br	-	2.063	1.973	2.040	2.050
Ga_B - O	1.846	1.818	1.856	1.848	1.838
	1.864	1.815	1.793	1.765	1.768
	1.842	1.736	1.868	1.743	1.775
	1.838	-	-	-	-
NN Ba-O br	2.562*	2.700	2.728	2.815	2.626
	3.479*	2.756	2.773	3.236	3.326
	-	3.010	3.123	-	-
NN La-O br	2.549*	2.604	2.547	2.489	2.653
	2.587*	-	-	2.723	2.724
Ba'_{La} - O br	-	2.756	2.728	4.623	5.275
	-	4.797	6.737	5.092	5.586
	-	5.097	7.090	5.115	6.199
	-	7.752	7.611	7.594	7.297
	-	7.851	7.865	7.693	8.870
Ba'_{La} - V_O	-	4.421	2.350	4.726	2.791
	-	5.022	4.876	6.424	7.152
NN cation - cation	3.707	3.589	3.588	3.808	3.658
	3.707	3.840	3.851	3.852	3.810
	3.899	4.091	4.061	4.099	4.191
	4.908	4.106	4.203	4.118	4.221

* NN O ion is considered rather than O bridge.

Table SI2. Ga-O bond angles (deg.) from DFT.

	$LaBaGaO_4$	model 1	model 2	model 3	model 4
Ga_A - O br	97.99*	91.46	94.25	98.24	96.58
	103.41*	101.45	106.51	102.97	103.00
	104.31*	135.56	121.21	107.79	122.51
Ga_A - O	108.81	103.04	108.25	112.42	108.59
	111.26	107.28	111.02	115.52	112.16
	130.13	118.86	113.17	117.36	113.19
Ga_B - O br	-	102.58	100.25	93.35	95.51
	-	103.06	102.59	100.04	101.55
	-	112.52	131.68	140.30	129.55
Ga_B - O	-	111.52	109.93	100.64	102.73
	-	111.87	110.54	105.60	110.97
	-	114.35	100.96	118.01	116.49

* NN O ion is considered rather than O bridge.