Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials: First-Principles Study of Li-Aluminosilicate Glass Scintillators

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Table S1:

Calculated electronic band gap E_g, valence band maximum E_{VBM}, conduction band minimum E_{CBM} and obtained glass densities for 20 configurations of each glass compositions. In red, experimental values from Tyrrell [1].

Glass Model	GS2				GSR1				GSR2			
	E_g (eV)	E_{VBM} (eV)	E_{CB} (eV)	ρ (g/cm^3)	E_g (eV)	E_{VBM} (eV)	E_{CB} (eV)	ρ (g/cm^3)	E_g (eV)	E_{VBM} (eV)	E_{CB} (eV)	ρ (g/cm^3)
1	1.924	4.008	5.932	2.77	3.041	2.088	5.129	2.35	2.272	2.747	5.019	2.61
2	1.468	4.014	5.482	2.74	2.563	2.637	5.2	2.34	2.209	3.562	5.771	2.57
3	2.569	3.181	5.75	2.72	2.897	2.945	5.842	2.56	3.195	2.465	5.66	2.57
4	2.889	3.045	5.934	2.73	2.274	2.622	4.896	2.40	2.577	2.579	5.156	2.54
5	2.076	3.879	5.955	2.76	2.55	3.037	5.587	2.44	2.731	2.383	5.114	2.49
6	2.403	2.837	5.24	2.59	2.718	2.799	5.517	2.48	2.363	2.978	5.341	2.43
7	2.389	3.916	6.305	2.85	2.576	3.378	5.954	2.56	2.689	3.043	5.732	2.58
8	2.738	3.293	6.031	2.80	2.389	3.301	5.69	2.49	2.38	3.135	5.515	2.48
9	2.569	3.369	5.938	2.76	2.572	3.176	5.748	2.50	3.023	2.898	5.921	2.63
10	2.578	3.261	5.839	2.70	2.218	3.129	5.347	2.40	3.028	2.36	5.388	2.46
11	2.404	3.073	5.477	2.65	2.24	3.203	5.443	2.51	2.585	1.864	4.449	2.41
12	1.733	3.911	5.644	2.66	2.244	3.005	5.249	2.48	2.716	2.826	5.542	2.54
13	2.065	3.481	5.546	2.67	2.711	2.952	5.663	2.49	2.221	3.376	5.597	2.55
14	3.09	3.018	6.108	2.82	2.557	2.849	5.406	2.45	2.699	2.593	5.292	2.47
15	2.223	3.389	5.612	2.67	2.755	2.639	5.394	2.50	3.018	2.326	5.344	2.48
16	2.58	3.287	5.867	2.75	2.073	2.93	5.003	2.46	2.839	2.985	5.824	2.60
17	2.103	3.599	5.702	2.71	2.708	2.661	5.369	2.39	3.169	2.382	5.551	2.51
18	1.918	3.833	5.751	2.71	2.362	3.047	5.409	2.43	1.955	2.987	4.942	2.62
19	1.916	3.963	5.879	2.74	2.74	3.121	5.861	2.54	2.227	3.275	5.502	2.49
20	1.929	3.948	5.877	2.75	2.773	2.265	5.038	2.48	2.331	2.671	5.212	2.52
Average	***2.281***	***3.515***	***5.793***	***2.73 (2.66)***	***2.548***	***2.8892***	***5.437***	***2.46***	***2.611***	***2.771***	***5.393***	***2.53***
Std dev.	***0.092***	***0.087***	***0.055***	***0.014***	***0.057***	***0.074***	***0.067***	***0.014***	***0.08***	***0.093***	***0.078***	***0.014***

[1] G.C. Tyrrell, Phosphors and scintillators in radiation imaging detectors, Nucl Instrum Methods Phys Res A. 546 (2005) 180–187. https://doi.org/https://doi.org/10.1016/j.nima.2005.03.103.