Electronic Supplementary Material (ESI) for Materials Advances.

Chemical structure and dissolution behaviour of CaO and ZnO containing alkali-borosilicate glass: Supplementary Material

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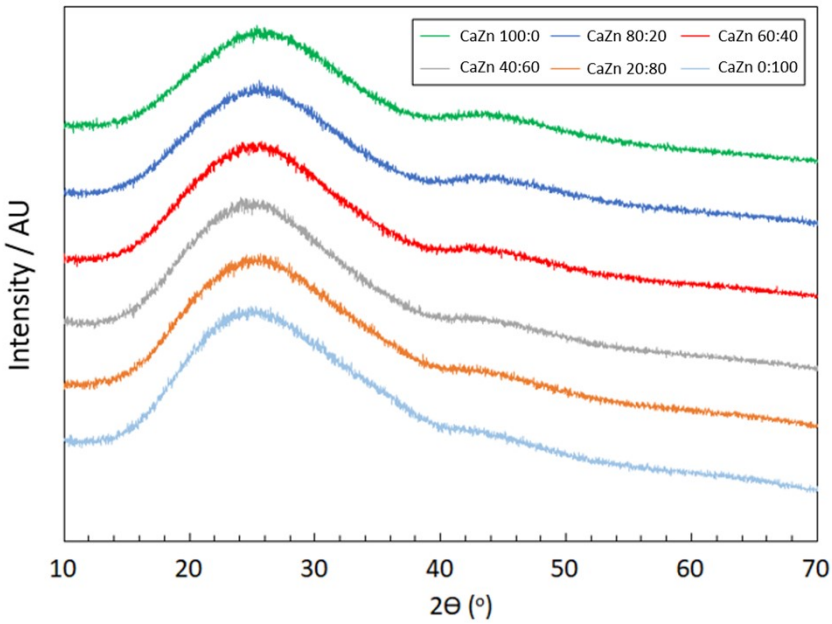
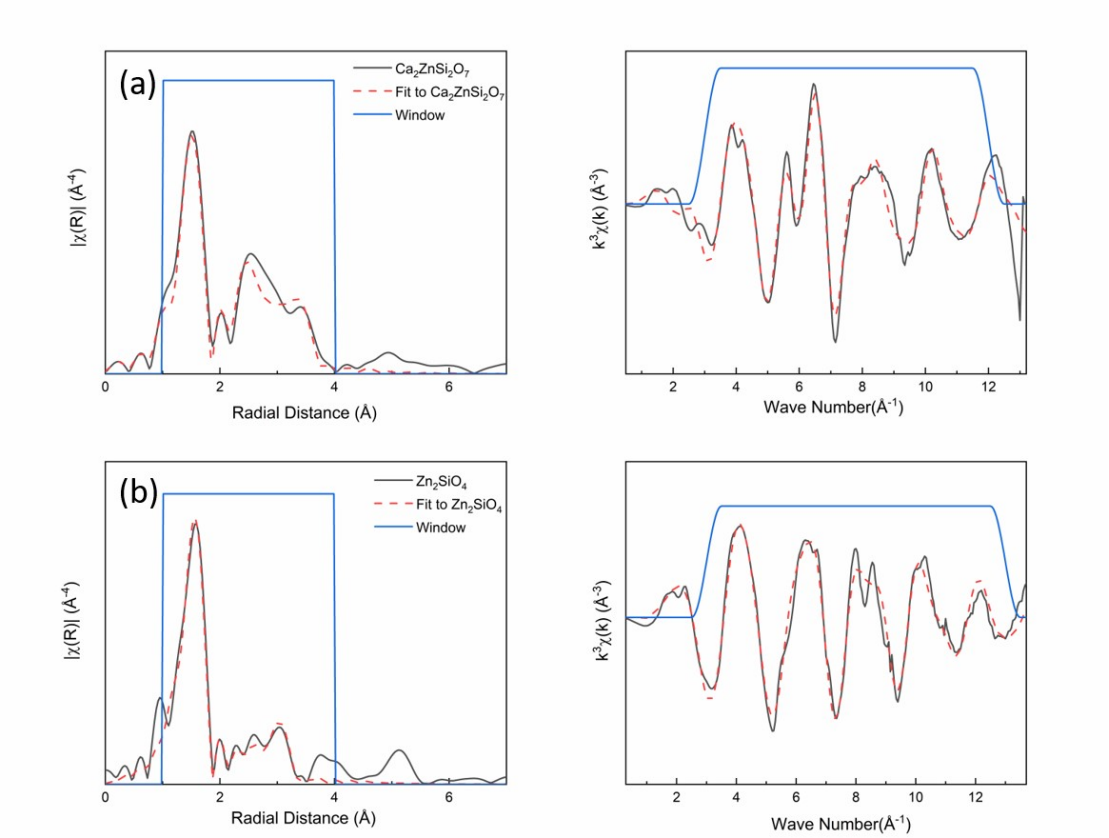


Supplementary Figure 1. X-ray Diffraction patterns acquired for the pristine Ca_xZn_y lithium alkali-borosilicate glass series.



Supplementary Figure 2. Extended X-ray Absorption Fine Structure (EXAFS) spectrum in radial space and the corresponding k^3- weighted EXAFS for Zn-containing standards: (a) hardystonite ($Ca_2ZnSi_2O_7$) and; (b) willemite (Zn_2SiO_4).

Supplementary Table 1. Peak assignments and fitting shapes for ^{11}B MAS NMR spectra used for the Ca_xZn_y glass series.

Coordination	Peak	Chemical shift / ppm	Fitting shape	Comments
$^{[3]}B$	(a) ring	16.8 (approx)	Q_{mas} 1/2	Amplitude, width and chemical shift (ppm) were refinable.
	(b) non-ring	14.5 (approx)	Q_{mas} 1/2	
$^{[4]}B$	(a) (1B, 3Si)	-1 (approx)	Gaussian	Amplitude, chemical shift (ppm), apodisation of theroretical lineshape, quadrupolar frequency were refinable. Asymmetry parameter (η_Q) was fixed.
	(b) (0B, 4Si)	-2.2 (approx)	Gaussian	

Equations used for ^{29}Si and ^{11}B MAS NMR spectral deconvolution:

$$R_{eff} = \frac{\left[(Na_2O) + (Li_2O) + (CaO)\right] - \left[(Al_2O_3) + (ZnO)\right]}{(B_2O_3)} \quad \text{(S1)}$$

$$K = \frac{(SiO_2)}{(B_2O_3)} \quad \text{(S2)}$$

$$R_{max} = \frac{1}{2} + \frac{1}{16}K \quad \text{(S3)}$$

$$R_{d1} = \frac{1}{2} + \frac{1}{4}K \quad \text{(S4)}$$

$$R_{dl2} = 2 + K \quad \text{(S5)}$$

The fraction of $^{[4]}$B was calculated considering the following:

$$^{[4]}\text{B} = \frac{8+K}{12}\left(1 - \frac{R_{eff}}{2+K}\right) \quad \text{if} \quad R_{d1} < R_{eff} < R_{d2}, \quad \text{(S6)}$$

$$^{[4]}\text{B} = R_{max} \quad \text{if} \quad R_{max} < R_{eff} < R_{d1}, \quad \text{(S7)}$$

$$^{[4]}\text{B} = R_{eff} \quad \text{if} \quad R_{eff} < R_{max.} \quad \text{(S8)}$$

The predicted $^{[3]}$B fraction is therefore given in Eqn. S9, and the comparison between the predicted $^{[4]}$B /$^{[3]}$B contributions and those measured by ^{11}B MAS NMR is given by Eqn. S10.

$$^{[3]}\text{B} = 1 - {}^{[4]}\text{B} \quad \text{(S9)}$$

$$B_{Accuracy} = \frac{B\ Measured}{B\ Predicted} \quad \text{(S10)}$$