Electronic Supplementary Material (ESI) for Dalton Transactions.

The corrosion behavior of borosilicate glass in the presence of cementitious waste forms

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SUPPLEMENTARY MATERIALS

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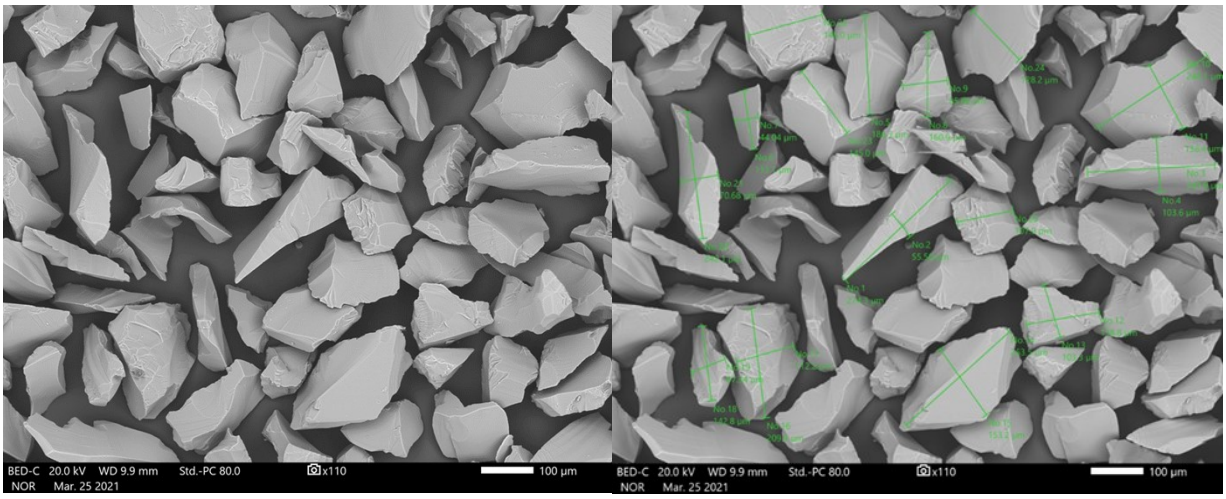


Fig. S1 Glass powder is prepared by crushing bulk glass. The glass was crushed with agate mortar and pestle, then sieved/washed. The average particle size is -100 to +200 mesh or 74–149 µm.

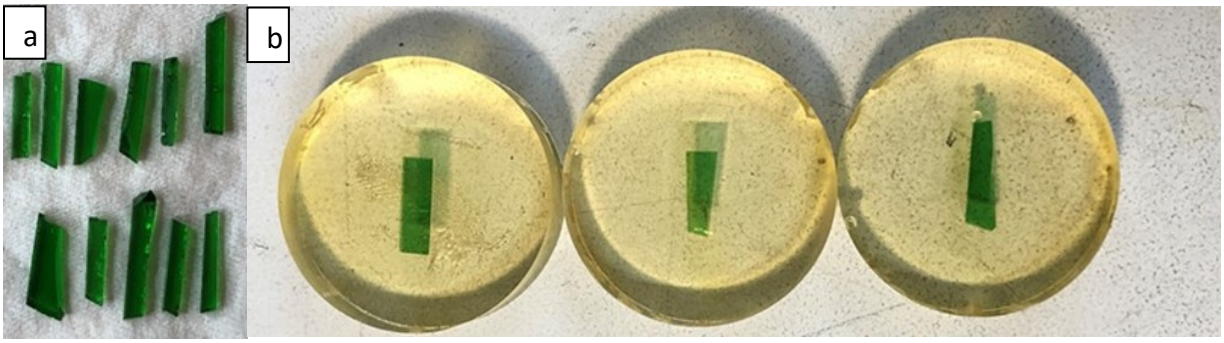


Fig. 2S (a) Glass coupons cut and polished for the glass characterization studies via SEM/EDS after the static experiment at 90°C; and (b) glass coupons mounted in epoxy resin and polished for cross-sectional SEM/EDS analysis.

Table S1. The composition of solutions measured in the PCT reactors is used for speciation modeling. The initial composition of the prepared leachate solutions is presented in Table 3.

Elements	***pH12***	***Si***	***Grout***	***Ca***	***Ca+Si***	***Al+Si***	***Ca+Si +Al***
	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
B	48,617.4	49,722.5	3,857.5	2,616.6	3,679.0	44,697.4	5,937.5
Si	100,776.7	103,750.7	12,531.1	4,683.1	6,574.6	94,928.6	29,567.4
Ca	338.5	479.4	84,307.2	81,222.0	70,631.9	575.5	4683.1
Al	30,517.4	31,824.9	10,664.9	4,246.1	5,167.1	34,842.8	27,899.2
K	37,289.1	40,306.4	2,979.4	3,836.4	5,193.3	35,206.1	24,359.0

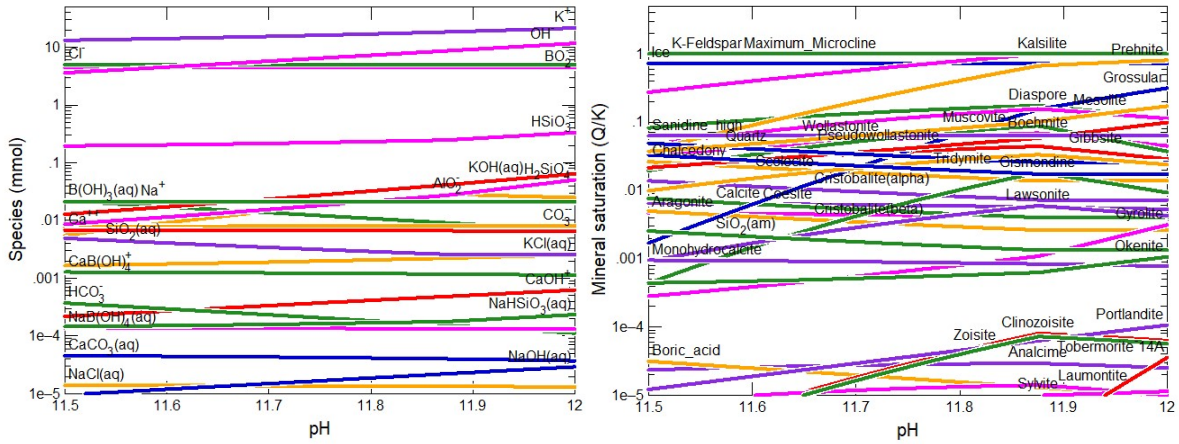


Fig. S3 Left) Aqueous speciation in control samples at pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

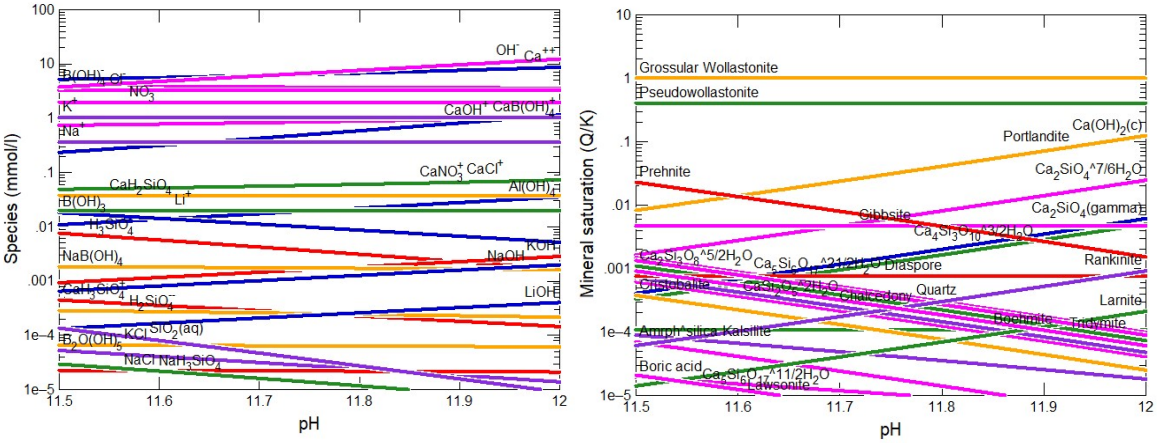


Fig. S4 Left) Aqueous speciation at the concentrations of ions present in the leachates with an initial Si- 0.18 mM (5 mg/L) and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

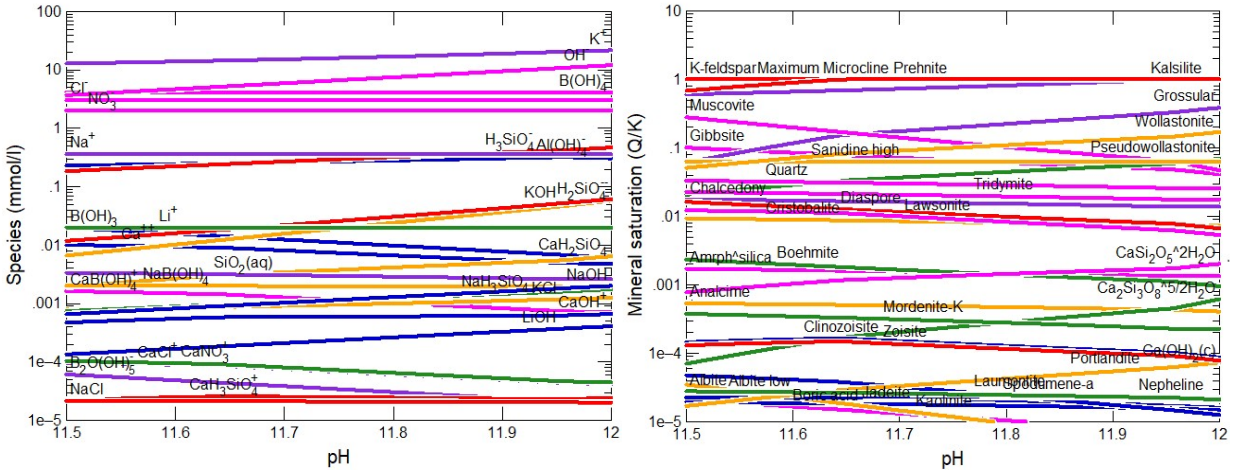


Fig. S5 Left) Aqueous speciation at the concentrations of ions present in the leachates, Si- 0.18 mM (5 mg/L), Al-0.26 mM (7 mg/L) and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

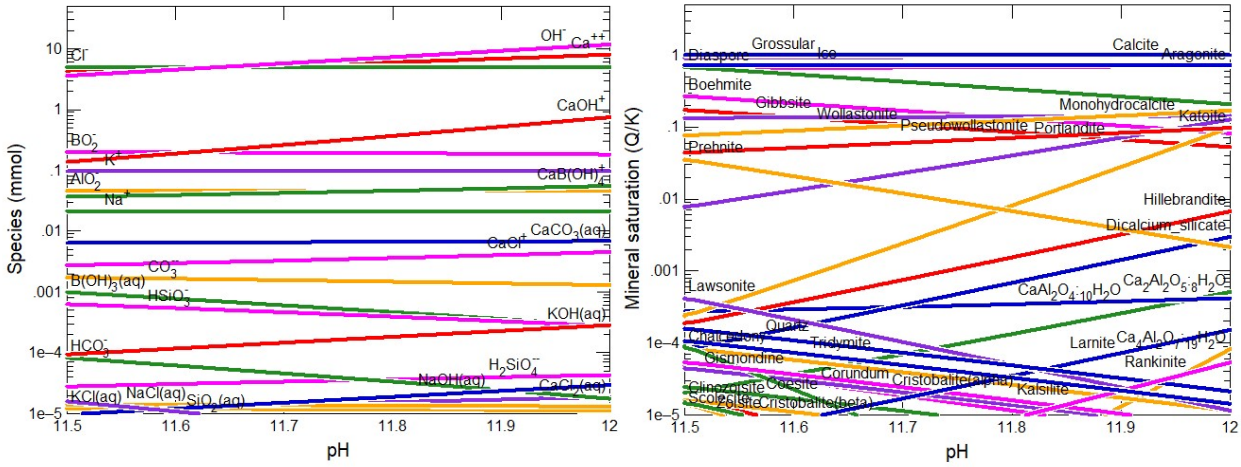


Fig. S6 Left) Aqueous speciation at the concentrations of ions present in the leachates, with initial Ca^{2+}-3.24 mM (130 mg/L and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

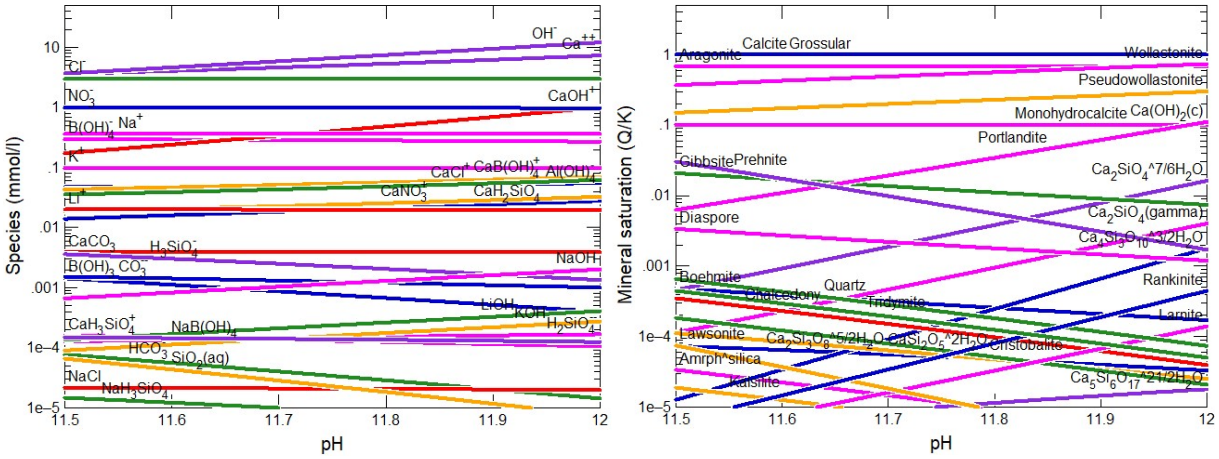


Fig. S7 Left) Aqueous speciation at the concentrations of ions present in the leachates, with initial solution concentrations of Si- 0.18 mM (5 mg/L), Ca^{2+}-3.24 mM (130 mg/L) and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

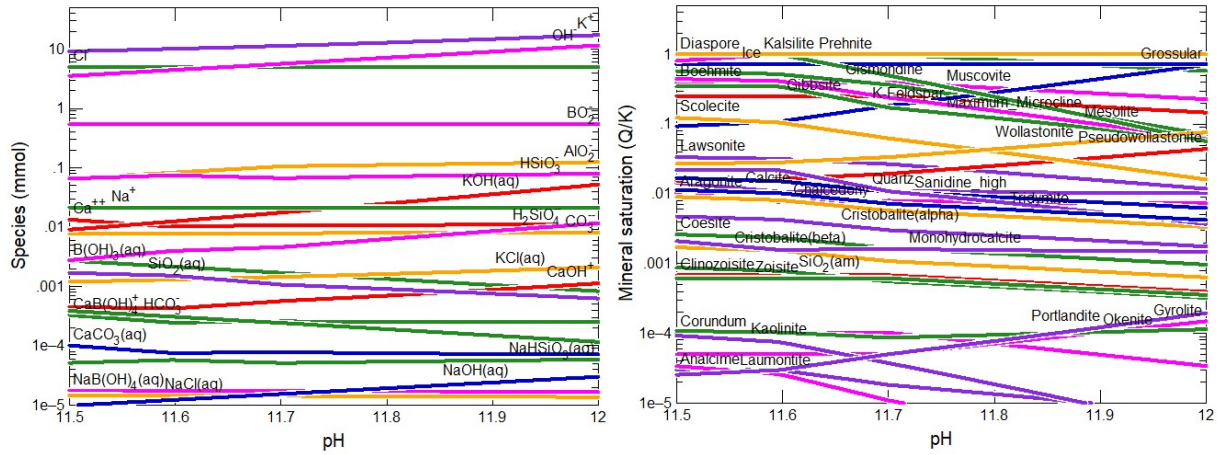


Fig.S8 Left) Aqueous speciation at the concentrations of ions present in the leachates with initial solution concentrations of Si- 0.18 mM (5 mg/L), Al-0.26 mM (7 mg/L), Ca^{2+}-3.24 mM (130 mg/L), and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.

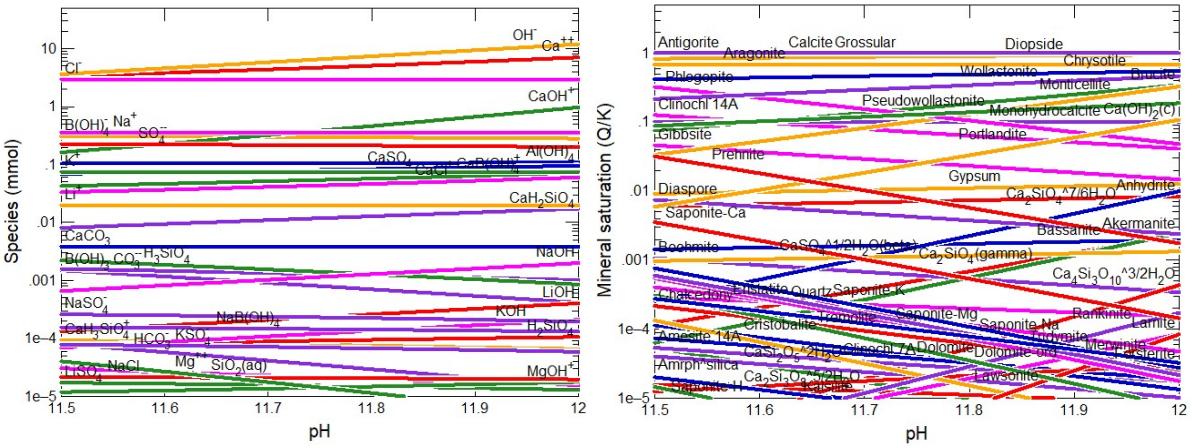
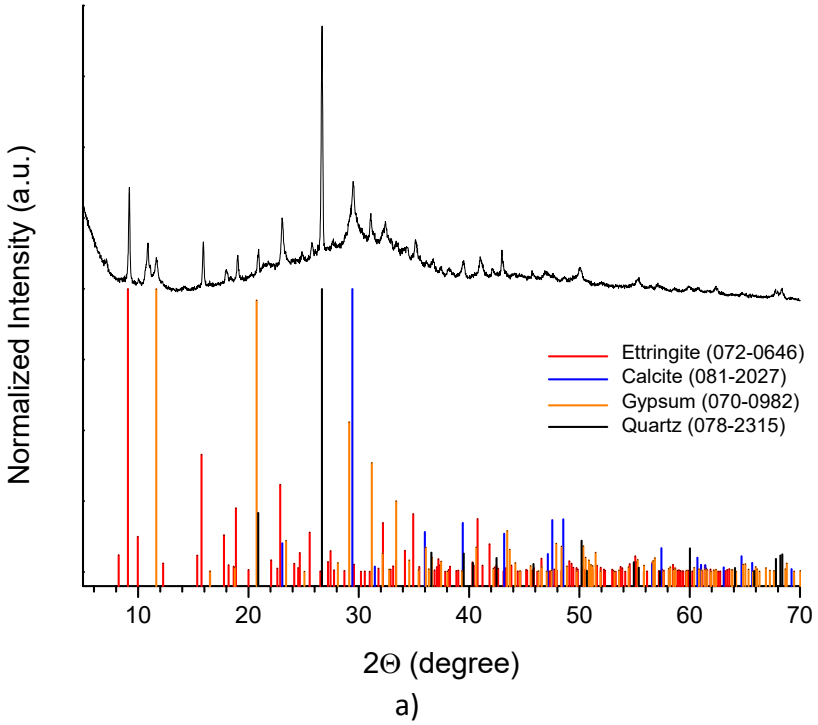


Fig.S9 Left) Aqueous speciation at the concentrations of ions present in the leachate of a grout-contacted solution and sliding pH in the range of 11.5 – 12.0; Right) Saturated indices of possible precipitates.



a)

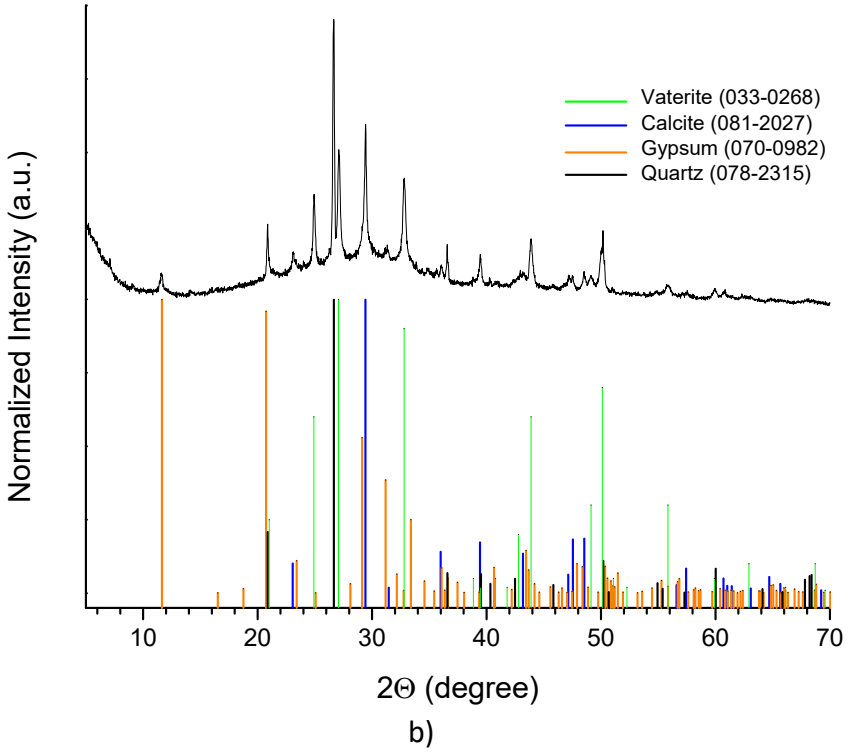


Fig. S10 (a) XRD patterns of as received and (b) water treated grout powders.

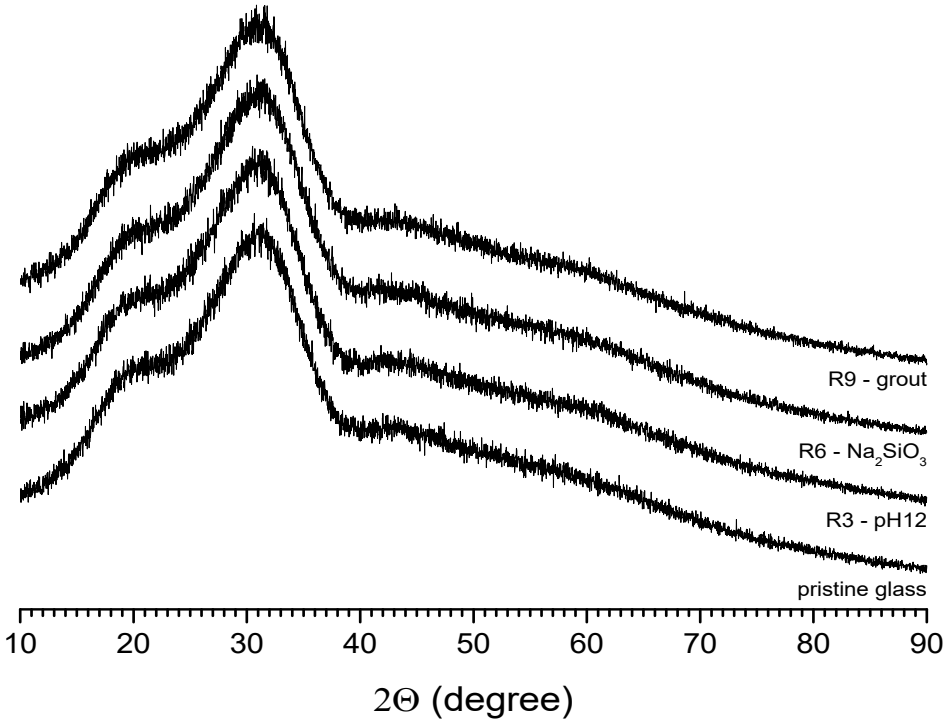


Fig. S11 XRD patterns of the powder pristine and treated glass in the static experiment at 90 °C.

Table S2 Phase composition of as received and water-contacted grout powders according to XRD analysis.

Phase	As received grout, wt. %	Water-contacted grout, wt. %
Calcite ($CaCO_3$)	11.1	17.0
Vaterite ($CaCO_3$)	0	52.0
Gypsum ($CaSO_4 \cdot 2H_2O$)	16.3	8.5
Quartz (SiO_2)	30.2	22.5
Ettringite ($Ca_6Al_2(SO_4)_3(OH)_{12} \cdot 26H_2O$)	42.3	0

Table S3 pH of solutions before and after static PCT

Solution	Initial pH	pH after static PCT
pH 12 buffer	11.95	11.73
Grout-contacted	11.78	11.64
Si-amended	11.94	11.73
Ca-amended	12.1	11.97
Ca- and Si-amended	12.13	11.85
Al- and Si-amended	12.01	11.79
Ca-, Al- and Si-amended	11.97	11.78

Table S4 Surface composition of pure glass powder and glass powders treated in pH 12 buffer, grout-contacted and Ca-amended solutions in PCT (7 days at 90°C) according to EDS analysis. Note: The average concentrations of elements were calculated based on the composition obtained from at least 10 single points.

Element	Pure glass wt. %	pH 12 buffer wt. %	Grout-contacted wt. %	Ca-amended wt. %
Magnesium (MgO)	0.39 ± 0.23	0.43 ± 0.1	0.44 ± 0.1	0.42 ± 0.1
Aluminum (Al_2O_3)	4.38 ± 0.66	4.77± 0.4	4.98 ± 0.3	4.78 ± 0.6
Silicon (SiO_2)	19.81± 1.72	21.18 ± 1.5	20.23 ± 1.2	20.45 ± 1.8
Calcium (CaO)	2.69 ± 0.97	2.30 ± 0.5	2.07 ± 0.6	2.73 ± 0.7
Iron (Fe_2O_3)	0.54 ± 0.20	0.56 ± 0.2	0.55 ± 0.3	0.55 ± 0.1
Sodium (Na_2O)	10.83 ± 2.57	8.97 ± 1.3	12.06 ± 1.4	9.96 ± 2.3
Potassium (K_2O)	0.86 ± 0.30	0.62 ± 0.1	0.72 ± 0.3	0.70 ± 0.2
Zinc (Zn)	2.24 ± 1.65	2.58 ± 1.4	2.33 ± 1.0	1.48 ± 1.2
Zirconium (ZrO_2)	7.59 ± 1.51	7.72 ± 0.5	6.89 ± 0.8	6.95 ± 0.3
Titanium (TiO_2)	0.50 ± 0.26	0.45 ± 0.1	0.41 ± 0.2	0.53 ± 0.53
Boron (B_2O_3)	11.70 ± 2.69	13.17 ± 2.6	12.60 ± 2.1	12.99 ± 1.7