

Supporting Information

for

Revealing the effect of anions on the formation and transformation of Zeolite LTA

in caustic solutions:

an *in-situ* synchrotron PXRD study

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Figure Lists

Fig.S1 3D X-ray diffraction patterns collected during the time-resolved in-situ PXRD experiments showing transformations between zeolite minerals in (a) 4 M NaOH; (b) 8 M NaOH; (c) 4 M NaOH with 0.1 M Na₃PO₄; (d) 8 M NaOH with 0.1 M Na₃PO₄; (e) 4 M NaOH with 0.1 M Na₂CO₃; (f) 8 M NaOH with 0.1 M Na₂CO₃; (g) 4 M NaOH with 0.1 M Na₂SO₄; (h) 8 M NaOH with 0.1 M Na₂SO₄. LTA: zeolite LTA; SOD: sodalite.

Fig.S2 Particles of zeolite LTA and sodalites after the ex-situ quench experiments at 90°C under conditions of (a): 4 M NaOH; (b): 4 M NaOH with 0.1 M Na₂CO₃; (c): 4 M NaOH with 0.1 M Na₂SO₄; (d): 4 M NaOH with 0.1 M Na₃PO₄; (e): 8 M NaOH; (f): 8 M NaOH with 0.1 M Na₂CO₃; (g): 8 M NaOH with 0.1 M Na₂SO₄; (h): 8 M NaOH with 0.1 M Na₃PO₄.

Fig.S3 Curve fittings for the in-situ time-resolved experimental data based on kinetic rate equations (1) or (2). Note the rate constants (Table 2) were obtained by fitting the kinetic data of zeolite LTA under (a): 4 M NaOH; (b): 8 M NaOH; (c): 4 M NaOH with 0.1 M Na₂CO₃; (d): 8 M NaOH with 0.1 M Na₂CO₃; (e): 4 M NaOH with 0.1 M Na₂SO₄; (f): 8 M NaOH with 0.1 M Na₂SO₄; (g): 4 M NaOH with 0.1 M Na₃PO₄; (h): 8 M NaOH with 0.1 M Na₃PO₄. For experiments without sodalite formation, $f(x) = 1 - k_2 \cdot \exp(-k_1 \cdot x) / (k_2 - k_1) + k_1 \cdot \exp(-k_2 \cdot x) / (k_2 - k_1)$ was used for fitting. For experiments with sodalite formation, $f(x) = \exp(-k_1 \cdot x) \cdot (k_2 - k_3) - \exp(-k_2 \cdot x) \cdot (k_1 - k_3) + \exp(-k_3 \cdot x) \cdot (k_1 - k_2)$ was used for fitting.

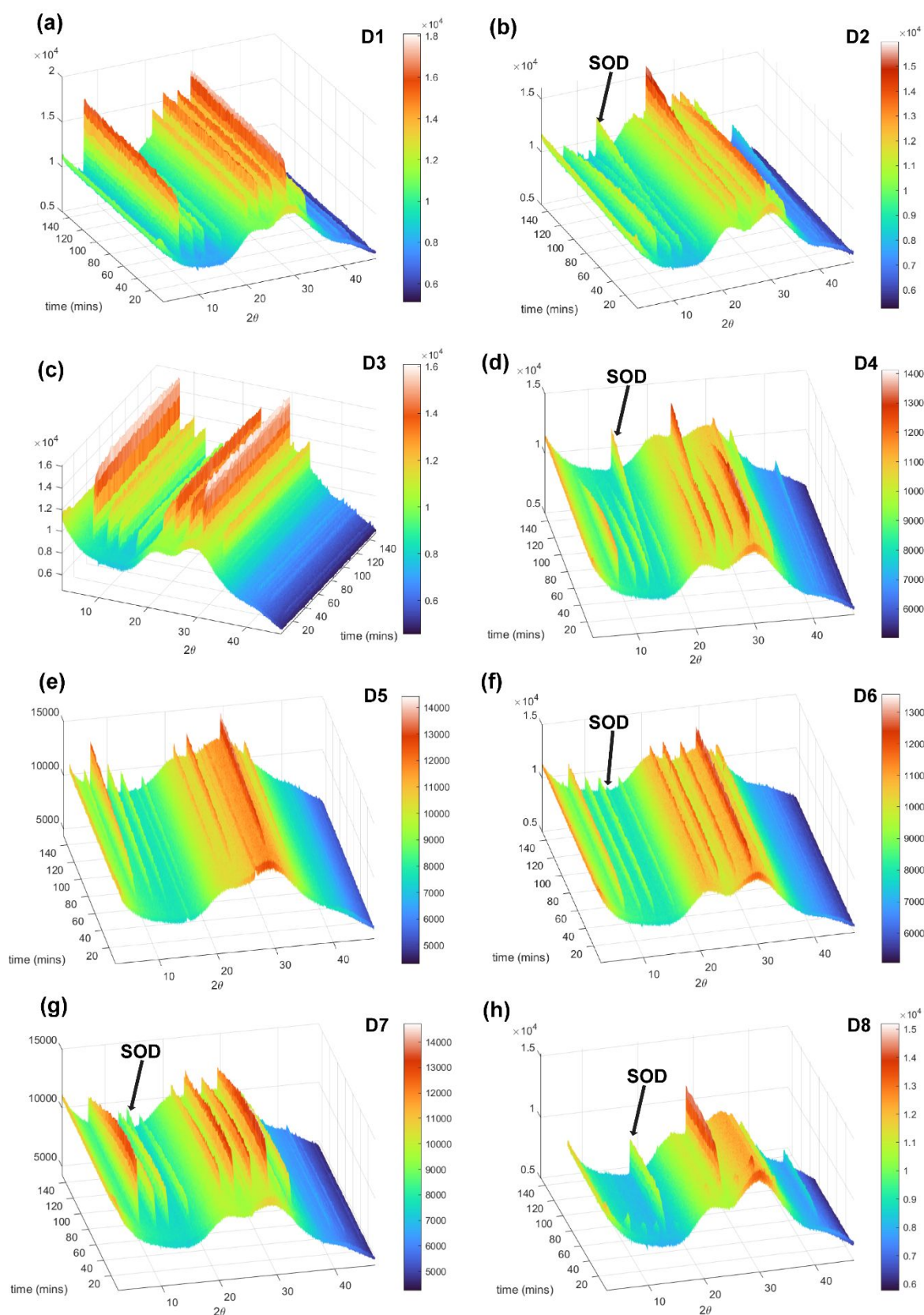


Fig.S1 3D X-ray diffraction patterns collected during the time-resolved in-situ PXRD experiments showing transformation between zeolite minerals in (a) 4 M NaOH; (b) 8 M NaOH; (c) 4 M NaOH with 0.1 M Na_3PO_4 ; (d) 8 M NaOH with 0.1 M Na_3PO_4 ; (e) 4 M NaOH with

0.1 M Na_2CO_3 ; (f) 8 M NaOH with 0.1 M Na_2CO_3 ; (g) 4 M NaOH with 0.1 M Na_2SO_4 ; (h) 8 M NaOH with 0.1 M Na_2SO_4 .

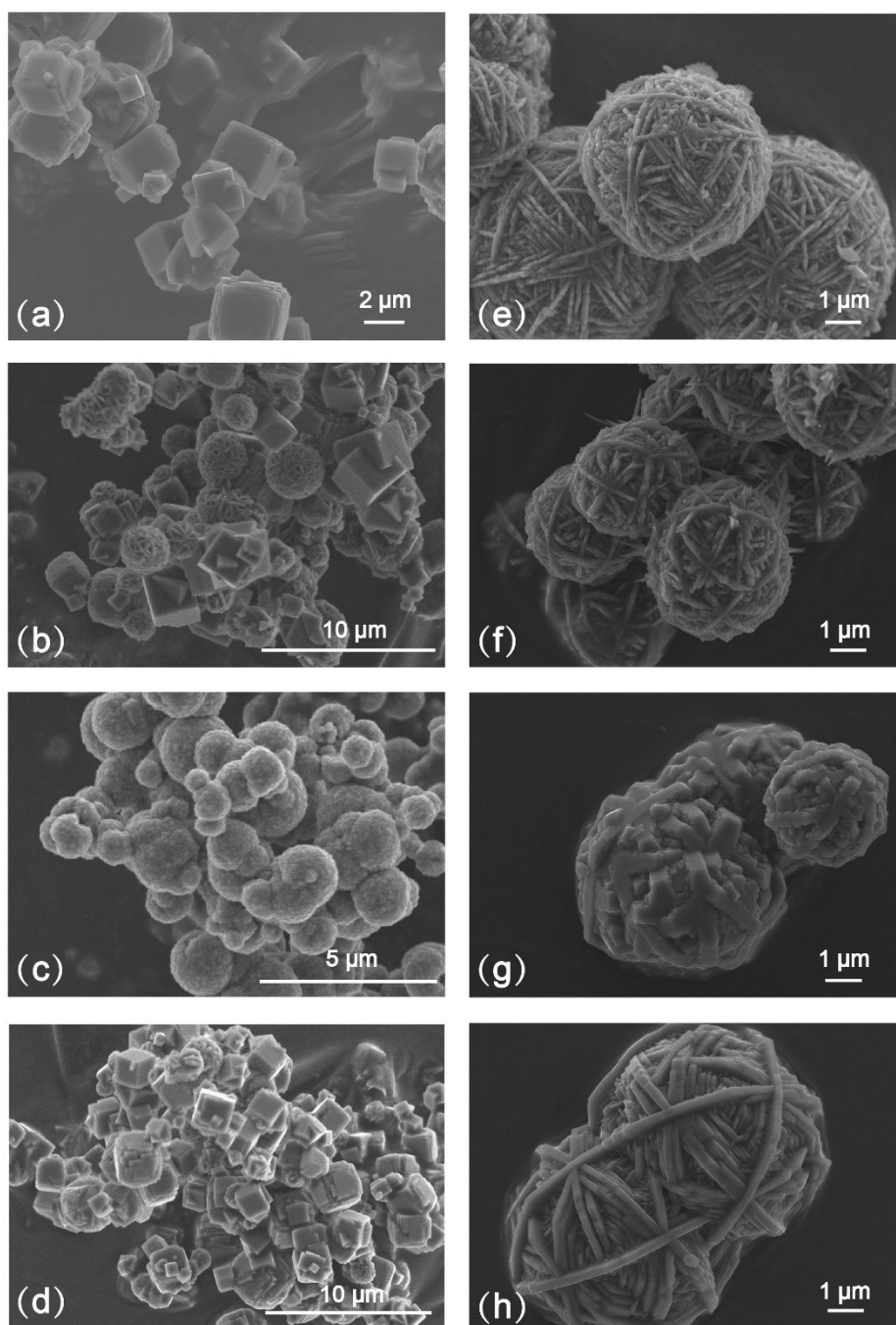


Fig.S2 Particles of zeolite LTA and sodalites after the ex-situ quench experiments at 90°C under conditions of (a): 4 M NaOH; (b): 4 M NaOH with 0.1 M Na_2CO_3 ; (c): 4 M NaOH with 0.1 M Na_2SO_4 ; (d): 4 M NaOH with 0.1 M Na_3PO_4 ; (e): 8 M NaOH; (f): 8 M NaOH with 0.1 M Na_2CO_3 ; (g): 8 M NaOH with 0.1 M Na_2SO_4 ; (h): 8 M NaOH with 0.1 M Na_3PO_4 .

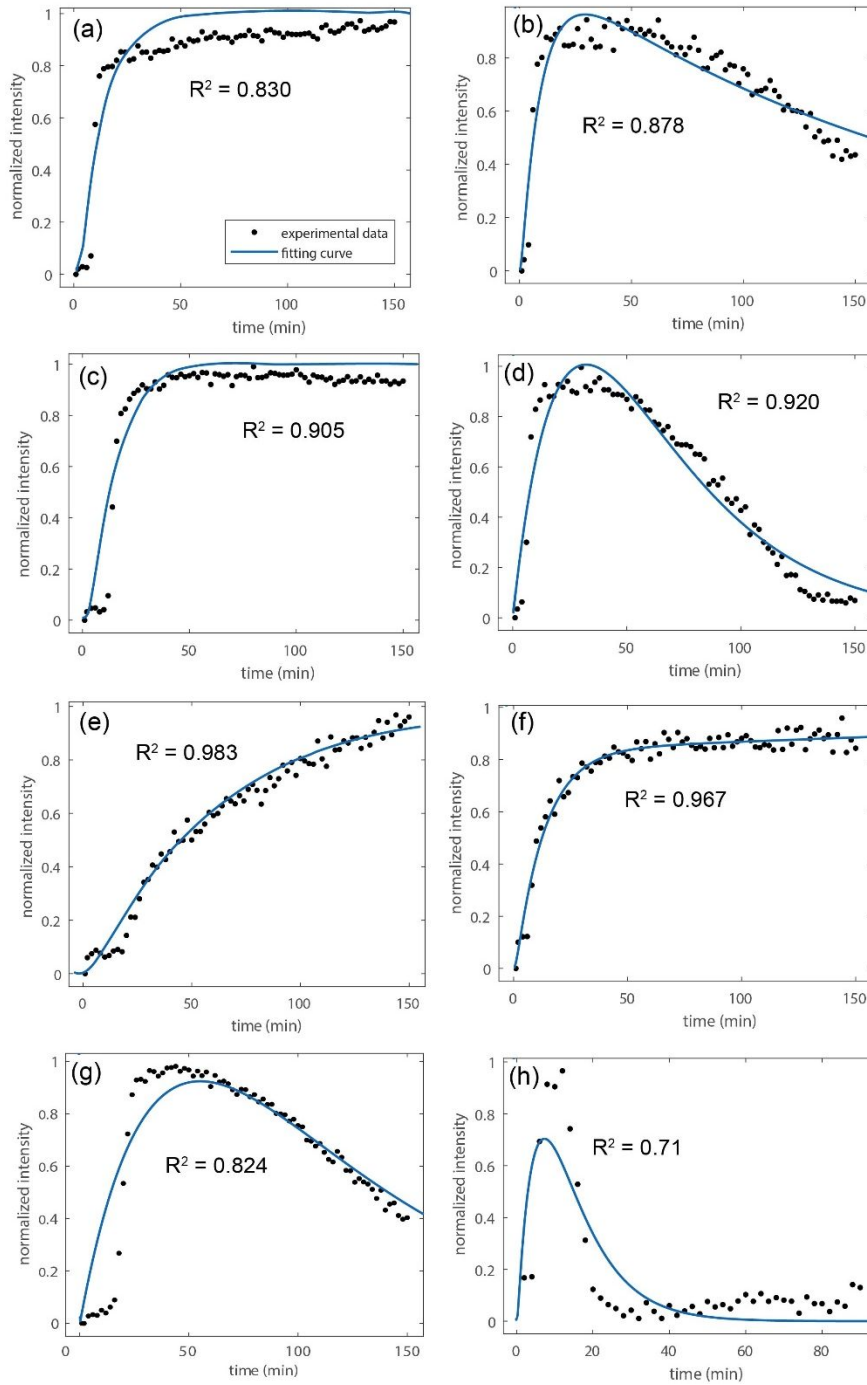


Fig.S3 Curve fitting for the in-situ time-resolved experimental data based on rate equations derived in section 2.3. Note the rate constants (Table 2) were obtained by fitting the kinetic data of zeolite LTA under (a): 4 M NaOH; (b): 8 M NaOH; (c): 4 M NaOH with 0.1 M Na₂CO₃; (d): 8 M NaOH with 0.1 M Na₂CO₃; (e): 4 M NaOH with 0.1 M Na₂SO₄; (f): 8 M NaOH with 0.1 M Na₂SO₄; (g): 4 M NaOH with 0.1 M Na₃PO₄; (h): 8 M NaOH with 0.1 M Na₃PO₄. For experiments without sodalite formation, $f(x) = 1 - k_2 \cdot \exp(-k_1 \cdot x) / (k_2 - k_1) + k_1 \cdot \exp(-k_2 \cdot x) / (k_2 - k_1)$ was used for fitting. For experiments with sodalite formation, $f(x) = \exp(-k_1 \cdot x) \cdot (k_2 - k_3) - \exp(-k_2 \cdot x) \cdot (k_1 - k_3) + \exp(-k_3 \cdot x) \cdot (k_1 - k_2)$ was used for fitting.