

Supplementary information

Local concentration controls the hydrate phase of calcium oxalate

Zhaodong Wang, Lala Du, Qihang Wang, Jingjing Xie, Zhengyi Fu, and Zhaoyong Zou*

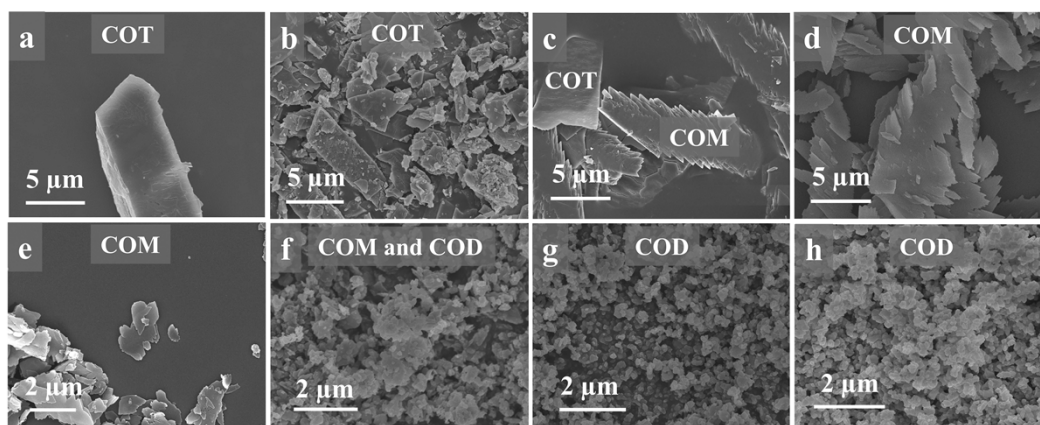


Figure S1. SEM images of samples collected after obtained after 10 min reaction for “calcium to oxalate” reaction at various concentrations: (a) 0.625mM, (b) 1.25mM-C1, (c) 1.25mM-C2, (d) 2.5mM, (e) 5 mM, (f) 10 mM, (g) 20 mM, (h) 40 mM.

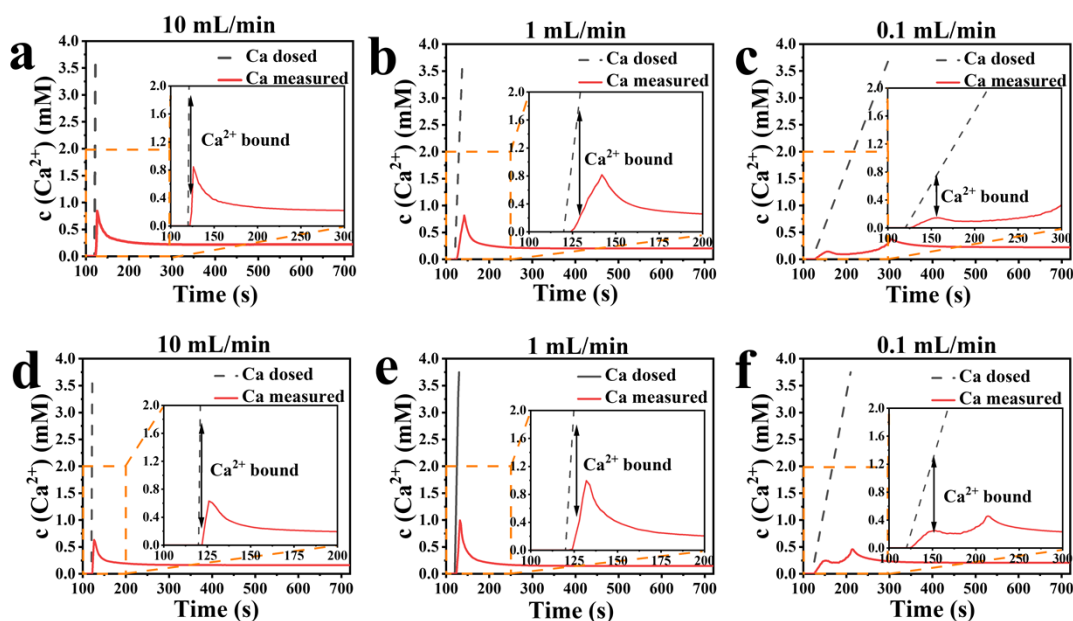


Figure S2. Curves of Ca²⁺ concentration for reaction with (a-c) 1 M and (d-f) 0.5 M CaCl₂ solution in titration equipment. (a, d) the titration rate is 10 mL/min, (b, e) the titration rate is 1 mL/min, and (c, f) the titration rate is 0.1 mL/min.

Calculations of the supersaturation

The ionic strength and supersaturation were calculated according to the literature¹.

Briefly, the ionic strength (I) is calculated according to formula S1. The activity coefficient (γ) is calculated according to formula S2. The activity is calculated according to formula S3. The supersaturations with respect to various phases are then calculated according to formula S4.

$$I = \frac{1}{2} \sum_{i=1}^n c_i Z_i^2 \quad \text{Formula S1}$$

$$\text{Log}(\gamma_i) = 0.5 \cdot Z_i^2 \left(\frac{\sqrt{I}}{1 + Ba\sqrt{I}} - 0.2 \cdot cI \right) \quad \text{Formula S2}$$

$$a_i = \frac{c_i}{\gamma_i} \quad \text{Formula S3}$$

$$S = \ln \frac{a_{Ca^{2+}} \cdot a_{Ox^{2-}}}{K_{sp}} \quad \text{Formula S4}$$

Reference

1. H. Werner, S. Bapat, M. Schobesberger, D. Segets and S. P. Schwaminger, *ACS Omega*, 2021, **6**, 26566-26574.