Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Nickel as a Modifier of Calcium Oxalate: An In-Situ Liquid Cell TEM Investigation of Nucleation and Growth

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Supplementary Video Captions:

Video S1. Growth of calcium oxalate trihydrate (COT) nanoparticle (NP) in presence of nickel ions.

Video S2. Atomistic molecular dynamics simulation of [CaOx] = 30 mM and [Ni] = 0 mM.

Video S3. Atomistic molecular dynamics simulation of [CaOx] = 30 mM and [Ni] = 4 mM.

Supplementary Figures:

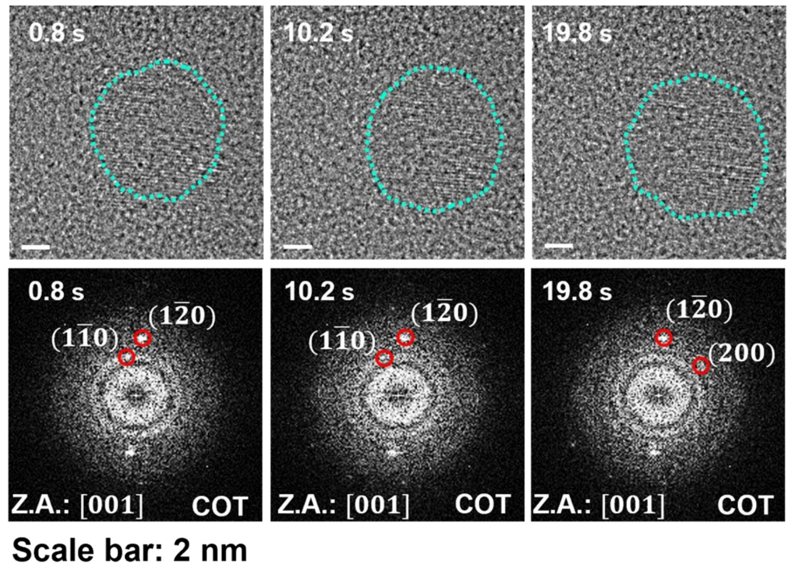

Figure S1. Time-lapse TEM micrographs and corresponding FFTs show no changes in phase and size of a COT nanoparticle acquired after 300 seconds of beam off.

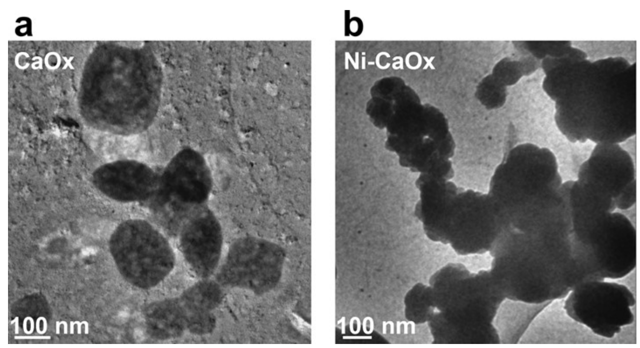

Figure S2. TEM micrographs of calcium oxalate nanoparticles formed in the absence (a) and presence (b) of nickel ions.

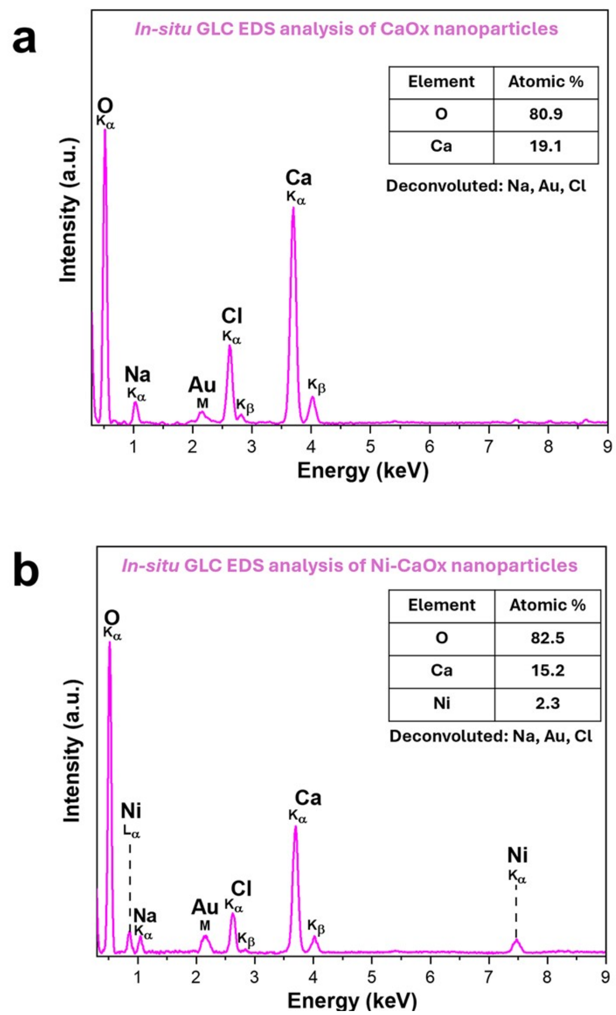

Figure S3. *In-situ* GLC EDS deconvoluted spectra of CaOx (a) and Ni-CaOx (b) nanoparticles. Deconvoluted elements include Au since the signal comes from Au grid and Na and Cl, which are spectator ions in the encapsulated solution.

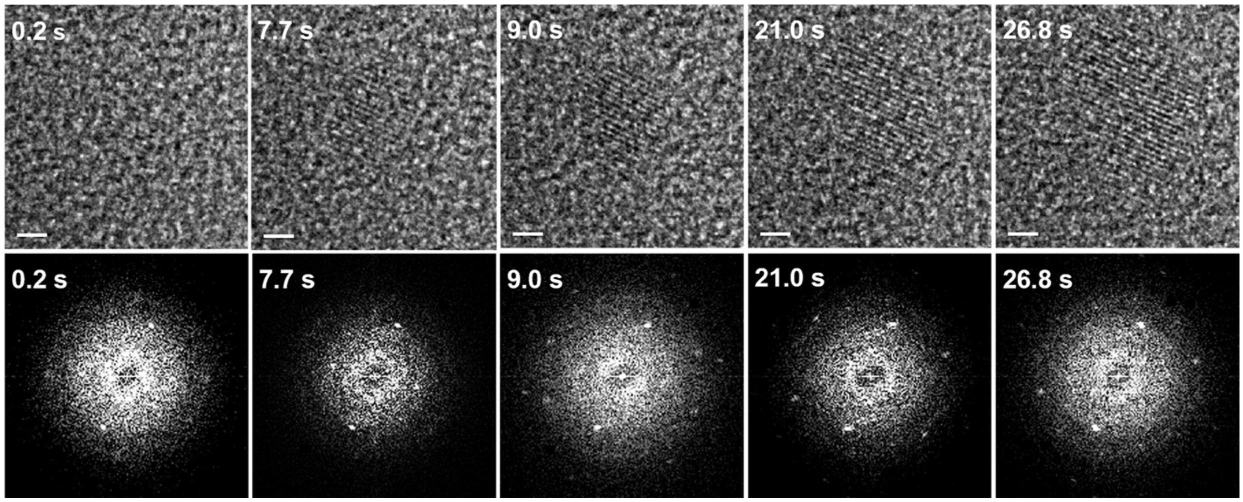

Figure S4. Time-lapse TEM micrographs and corresponding FFTs of a COT NP growing in the presence of Ni^{2+} ions. Scale bar: 2 nm.

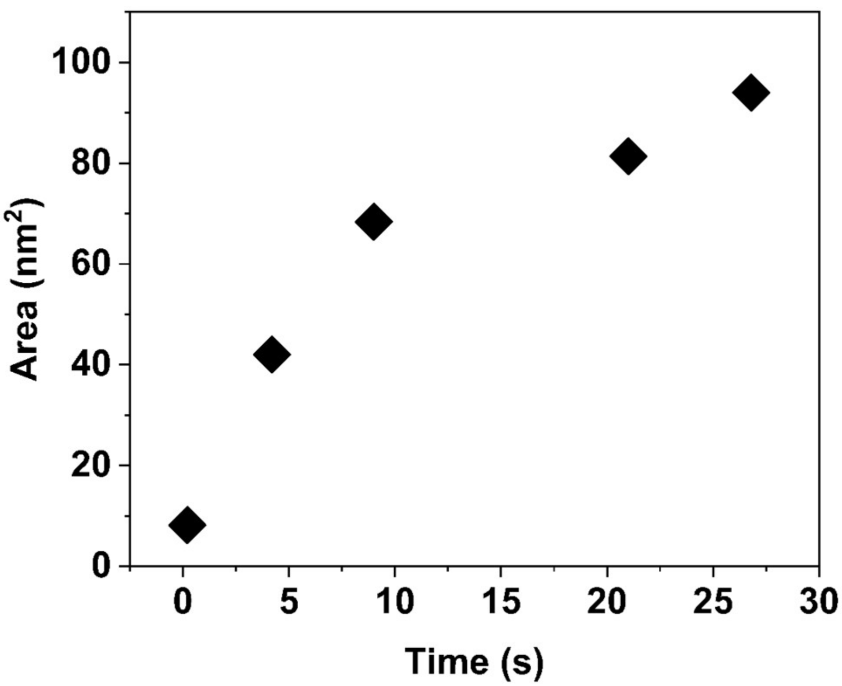

Figure S5. Change in area of a COT NP with Ni^{2+} over time.

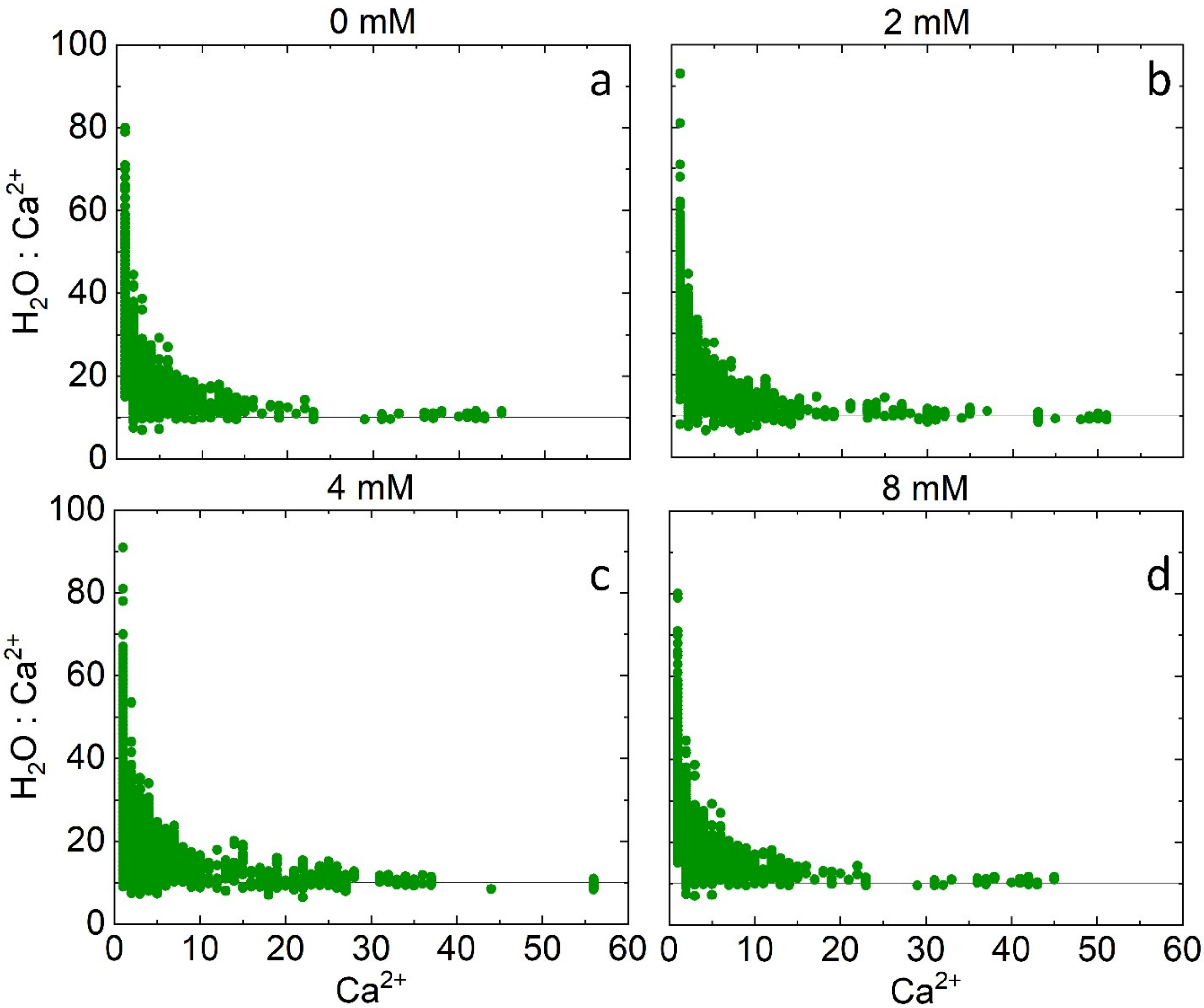

Figure S6. Number of water molecules within 4.5 Å per Ca^{2+} ion in a cluster vs. number of Ca^{2+} ion within a cluster at 0, 2, 4, and 8 mM concentrations.

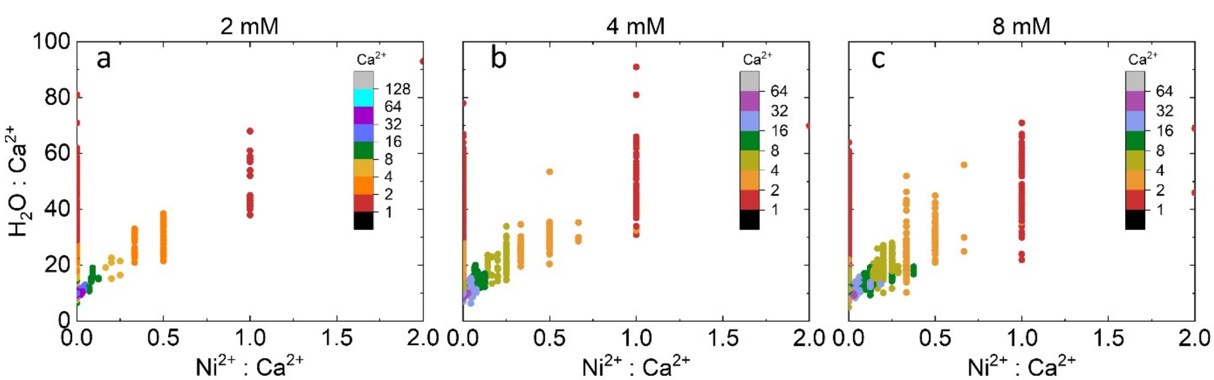

Figure S7. Number of water molecules within 4.5 Å per Ca^{2+} ion in a cluster vs. ratio of Ni^{2+} ions within 4.5 Å of a cluster with respect to number of Ca^{2+} ions in a cluster. Color scale shows the number of Ca^{2+} in cluster at 0, 2, 4, and 8 mM concentrations.

Supersaturation of calcium oxalate:

The degree of supersaturation in the control calcium oxalate sample was estimated using the following: [1, 2]

$$\sigma \approx \frac{c - c^{sat}}{c^{sat}} \qquad \text{(S1)}$$

$$\sigma \approx \frac{0.03\,M - 0.57 \times 10^{-4}\,M}{0.57 \times 10^{-4}\,M}$$

$$\sigma \approx 525$$

σ - the supersaturation of the CaOx solution

c - the concentration of the solute

c^{sat} - solute solubility

1. J. M. Schall, G. Capellades and A. S. Myerson, *CrystEngComm*, 2019, **21**, 5811-5817.
2. I. Gutzow, S. Atanassova, G. Budevsky and K. Neykov, *Urological research*, 1993, **21**, 181-185.