Supporting Information

Direct In Situ ATR-IR Spectroscopy of Structural Dynamics of NH₄H₂PO₄ in

Aqueous Solution

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Figure S1 Concentration dependent ATR-IR spectra of ADP solution.



Figure S2 pH dependent ATR-IR spectra of supersaturated ADP solution.



Figure S3 Time dependent ATR-IR spectra of ADP supersaturated solution.



Figure S4. Time dependent peak height and peak area of vibrations of P–O (a,b), P–OH (c,d), P–O···H-O–P (e), and NH_4^+ (f) in ATR-IR spectra.



Figure S5. Time dependent FWHM of vibrations of P–O (a,b), P–OH (c,d), P–O···H-O–P (e), and NH_4^+ (f) in ATR-IR spectra.



Figure S6 Structural characteristics of ADP. (a) Unit cell of ADP. (b) Structural characteristics of {100} plane. (c) Structural characteristics of {101} plane.



Figure S7 Morphology evolution of ADP crystallites in aqueous solutions with different pH values, from (a) to (f), the corresponding pH values are 1.64, 3.30, 3.83, 4.24, 4.68 and 5.65, Scale bar = $200 \mu m$.



 $\sigma = 0.1$

 $\sigma = 0.2$

Figure S8 Morphology evolution of ADP crystals grown under different supersaturations. The samples were prepared by naturally evaporating ADP solution at room temperature.



Figure S9 Morphology evolution of ADP crystallites in aqueous solutions with different superstations, from (a) to (d), the corresponding superstation degrees are 0.05, 0.10, 0.20, 0.30, respectively. Scale bar = $200 \mu m$. ADP of analytical grade and deionized water are used in the present experiments, which are carried out at ambient temperature 26 °C. The supersaturated ADP solutions of 40 °C are prepared, respectively. After the temperature of the solutions is decreased to ambient, ADP solution of ~10 ml was filtrated and transferred into a 50 ml glass beaker with agitating by magnetic stirrer and evaporates at ambient temperature, lots of ADP crystallites are grown spontaneously.