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Nanoscale insights into the formation and breakdown of struvite – a sustainable phosphate mineral

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Struvite ($MgNH_4PO_4{\cdot}6H_2O$) is a widespread phosphate mineral that readily precipitates from supersaturated aqueous solutions at ambient pressure and temperature conditions. Such a spontaneous struvite formation often causes significant concern to waste water treatment plants due to scaling. The controlled crystallization of struvite, on the other hand, is an attractive route for nutrient recovery from waste waters because of its potential use as a sustainable fertiliser. Struvite is also an important reaction product during synthesis of Mg-phosphate binders, which are used in various niche applications in civil engineering and biomedicine (e.g., road repair, bone tissue regeneration). Thus, it not surprising that elucidating the mechanism and kinetics of crystallisation and the thermal stability of struvite are of great interest to many fields. However, crucial information about the nanoscale pathways of crystallization and decomposition are still lacking, even though such knowledge can be of great value, e.g., for optimizing the performance and handling of struvite-based products.

Here we present data from a study where we i) quantified the nucleation and growth of struvite from solution and ii) evaluated the nanostructural evolution during its subsequent thermal decomposition by using various state-of-the-art characterisation techniques (including *in situ* and time resolved synchrotron-based X-ray scattering). Our results indicate that struvite forms through a particle-mediated process that involves the fast precipitation of primary nanoparticles (~50 nm in size) that subsequently self-assemble and transform into crystalline struvite. We further show that the thermal decomposition of struvite at $T < 100°C$ leads to a high porosity (~0.28 cm^3/g) and a strong increase in surface area (from 1.5 to 300 m^2/g). The final material is an X-ray amorphous Mg-phosphate nanostructure with a very narrow pore size distribution of uniform, 3-5 nm wide pore channels.

Our findings have implications for the formation and use of struvite in multiple applications and could open up new avenues for designing nanostructured phosphate-based materials, e.g., for biomedical purposes.