

(Trans)formation of polymeric precursors: a critical gap in understanding mechanisms of iron oxyhydroxide mineral formation in aqueous systems

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Classical nucleation theory has proved an excellent framework to describe and predict the conditions under which (that is when, and where) different iron oxyhydroxide mineral phases may form in aqueous systems. However, we still lack a fundamental understanding of the how these minerals form at a detailed, mechanistic level. Apart from satisfying intellectual curiosity and expanding fundamental knowledge, detailed understanding of these processes would have great value in controlling and tailoring mineral formation to suit a wide range of potential applications.

Here, I discuss the potential importance of polymeric precursors in these processes, viewed through the solution chemistry-based conceptual framework developed by Jean-Pierre Jolivet [1], and with reference to non-classical nucleation paradigms (Figure 1) [2]. I focus particularly on highlighting key gaps in knowledge needed to effectively employ and evaluate such conceptual frameworks, and describe some promising experimental and computational approaches to address these gaps. I additionally present examples from my own research group and others over the past decade to illustrate the use of some of these approaches in attempting to resolve key details of the mechanisms for formation and transformation of polymeric precursors to iron oxyhydroxide minerals in aqueous systems.

[1] Jolivet (2000), *Metal Oxide Chemistry and Synthesis*, John Wiley & Sons.

[2] Lukić, Gebauer & Rose (2020), *Current Opinion in Colloid & Interface Science* 46, 114-127.

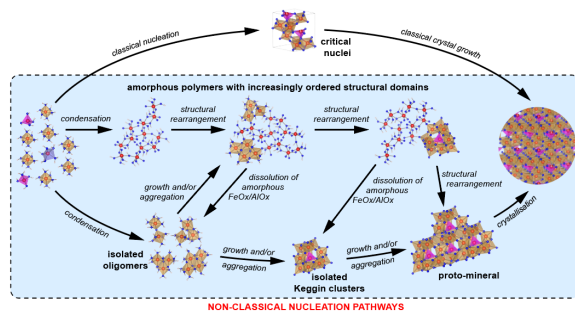


Figure 1 - Broad conceptual framework for pathways from solution phase to minerals for iron and aluminum oxyhydroxides in aqueous systems. Reproduced from [2].