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Understanding how organic molecules control mineral nucleation at the nanoscale

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Additives – small amounts of (organic) molecules – are known to be able to control the outcome of a crystallization process, even when present in minor quantities [*e.g.* 1-3]. Outcomes of these additive-mineral interactions are ubiquitous. Examples vary from biomineralization processes, such as the formation of skeletons, to a vast amount of industries being depended on organic-based crystallization additives in order to produce materials with tailored properties (e.g. approximately $20 billion/year are spent on cement additives). But, despite the pivotal role of organic molecules in the formation of (crystalline) materials taking place in natural and industrial environments, surprisingly little is known about their *modus operandi* at the nanoscale during the early stages of nucleation and growth [1]. We aim to correlate the physicochemical properties of model organic molecules with their functionality during the crystallization process of portlandite and calcium carbonate. To achieve this, we employ *in situ* time-resolved Pair Distribution Function (PDF) analyses combined with potentiometric titration measurements, as well as complementary *in situ* Small-Angle X-ray Scattering (SAXS) experiments to monitor the mineralization process in the presence of different types of organic molecules. In particular, our newly devised method for PDF pushes the resolution limit of what has been previously achieved in mineral nucleation studies from diluted solution. Our results suggest that different additives act on different stages of the portlandite nucleation process. This study will contribute to a better fundamental understanding of nucleation with and without additives and hence, serve as a step forward in biomineralization research as well as offer new insights for the development of sustainable crystallization additives in industry.

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