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Prenucleation clusters and calcium carbonate polyamorphism

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Nucleation of calcium carbonate from aqueous solution can follow an alternative pathway via stable pre-nucleation clusters [1], which is referred to as "non-classical nucleation", challenging the major concepts and assumptions underlying the classical nucleation theories [2]. Amorphous calcium carbonate (ACC), which is initially formed upon nucleation in this manner, exhibits distinct short-range structural features. Depending on pH, these structural characteristics can relate to the long-range order of different crystalline polymorphs of calcium carbonate [3], a phenomenon that is well-known from biominrealization. Recent results from computer simulation shed light on the atomistic background underlying non-classical nucleation of calcium carbonate [4]; they offer an explanation of the thermodynamic stability of pre-nucleation clusters, and rationalize the existence of a distinct barrier separating solution (pre-nucleation) and solution/solid (post-nucleation) states. Last, but not least, a possible foundation of different structures in precipitated ACC is suggested. The considerations show that the pre-nucleation cluster pathway may lead to a novel understanding of polymorph selection and control, not only in biomineralization, but also in geological, pharmaceutical or industrial contexts.

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