Molecular-level insight into the effects of amino acids on biomineralisation

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The incorporation of organic molecules into mineralised tissues lends these materials special mechanical properties. Furthermore, proteins directly influence the growth of mineral phases, controlling both the crystal structure and assembly of biominerals.

Calcium carbonate ($CaCO_3$) is often employed as a model system to investigate biomineralisation. In recent years, a number of nucleation and growth mechanisms have been proposed, which include the formation of stable clusters before nucleation [1], and the emergence of dense liquids, which are stabilised in the presence of polyASP [2,3]. An amorphous phase is known to precede crystalline $CaCO_3$ phases and it was shown that glycine-rich proteins stabilise this phase [4]. Picker *et al*. conducted an in depth study of the effect of all 20 amino acids on crystallization, identifying multiple effects on the stages of $CaCO_3$ crystallization [5]. The molecular level detail of this control remains obscure.

Here, we investigate the effect of three amino acids—ASP, ARG and GLY—on various stages of $CaCO_3$ growth using molecular dynamics with the Demichelis *et al*. force field [6]. Starting from dispersed ions in solution at 20 mM and pH 10, we investigated the effect of molecules on ionic speciation. We also simulated liquid-liquid phase separation in the presence of the amino acids, as well as the effect of surface-adsorbed molecules on the stability of amorphous $CaCO_3$. Our results suggest that amino acids can indeed regulate many aspects of biomineralisation, with evident changes to the stability of crystal precursor phases. Combined with experimental data, these new results offer important design principles for molecular additives to control mineral growth.

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