

Self-assembled monolayers as a model system for biomineralisation

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Self-assembled monolayers (SAMs) have long been used as substrates and/or templates for mineral growth[1] and as model systems for biomineralisation[2]. These organic systems provide arrays of organised head groups that can be functionalised and positioned to generate patterns and specific charge densities. How the water and ions within the solution organise at this interface is very important if we are to understand the mechanisms of nucleation and subsequent growth of minerals at this interface. Factors such as the surface concentrations of ions (which can be very different from that in the bulk), the flexibility of the SAM (i.e. strict epitaxial matching to a substrate may not be required) and the interfacial charge must be considered.

We explore models based on the Poisson-Boltzmann equation to obtain surface ion concentrations[3,4] and use these results in explicit all atom simulations[5,6] to examine the organisation and distribution of ions at these interfaces. Use of a constant chemical potential ensemble[7] allows us to accurately examine different ionic concentrations in atomic simulations that is normally not possible. We show that active surface defects affect the behaviour of ion clustering at the surface, which in turn affects the rate at which ionic clusters form and grow. We discuss the importance of structure and solution conditions at the interface on the efficacy of SAMs in controlling nucleation and growth pathways and hence the ability of SAMs to control which mineral polymorph is produced. Finally we relate the insights gained to possible mechanisms of biomineralisation.

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