Mineral-biomolecule binding and the mechanisms of biomineralisation

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Both biomineralisation and bioattachment involve an interface between minerals (hard) and biomolecules (soft). Such an interface can exercise control in two directions. First, the binding of large molecules on surfaces can induce conformational folding and consequent effects on molecular function. Understanding such reactions is essential for understanding the attachment of cells and bacteria (and consequently biofilms) to surfaces. On the other hand, soft matter can control the nucleation and growth of crystals. The resulting materials have complex structures, often with distinctive features at different lengthscales.

We will show how a combination of molecular dynamics simulations and experiment can shed light on the fundamental mechanisms of biomineralisation and the attachemnt of biomolecules. These examples will include the effect of binding on the stability of proteins in eggshells [1] and the implications for the survival of protein sequences into deep time; the effect of incorporating organic molecules into calcite on the crystal structure and properties [2] of the mineral; and methods by which biomolecules can control crystal nucleation and growth by biomolecules [3].

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