

## The structure-function relationship in bacteria

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What shape should a bacterium be? Intuitively, “The unity of bacterial cell design must play an important role in the ecologic success of prokaryotes. It is one that has lasted 3.5 billion years and, therefore, has survived the test of time” - Terry Beveridge. This ‘unity in cell design’ includes a diverse array of bacterial shapes and cell surface chemistries that bacteria have employed to produce their cell envelopes; their interface with their environment.

Examination of a Northam Pt mine biofilm using SEM and TEM demonstrated that it contained a morphologically diverse assortment of bacteria. The most unique and striking of these morphotypes were the ‘Stars’. The Stars are filamentous cells approx. 250 nm in diameter and up to 10 µm in length. The distinctive star shape is formed from longitudinal invaginations of the cell envelope and is best observed using ultrathin section transmission electron microscopy, which revealed the star shape.

The interface between bacteria and their environment is critical for both mineral formation and mineral dissolution processes. Laboratory experiments using *Desulfovibrio desulfuricans* and *Desulfotomaculum ruminis*, which contain different cell envelopes (i.e., gram negative vs. gram positive, respectively) demonstrated two strategies of mineral formation. TEM revealed that the nanophase FeS formed by *D. ruminis* was intimately associated with the bacterial cell surface. Aggregation of randomly oriented nanoparticles and XAFS indicated the cell wall influenced the nucleation and growth of these particles. In contrast, biogenic FeS formed by *D. desulfuricans* occurred as nanoparticles loosely associated with the gram-negative cell wall, which allowed them to rotate freely and grow via oriented aggregation.

The bacterial interface can now extend micrometers from the cell surface via the formation of bacterial nanowires, which allow for electron transfer processes to occur at some distance from the bacterium, protecting the cells from the toxic effect of heavy metals, e.g., gold [1], and enabling the cells to use solid phase electron acceptors.

[1] Lengke & Southam (2007) *Econ. Geol.* **102**, 109-126.

## The structure of water around Iron oxide mineral nanoparticles

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The interactions between water and mineral surfaces are crucial for stabilizing surface structures and mediating interfacial adsorption reactions of aqueous ions. Nanoscale minerals, such as the iron oxides, are extremely common natural products of biomineralization and chemical weathering reactions. Although frequently a minority volume fraction, mineral nanoparticles can have a profound impact due to their high surface areas, high reactivity and total energy relative to macroscopic minerals. The structure and chemistry of the water-nanoparticle interface is crucial in determining the transport of ions to the nanoparticle surface and its reactivity. Computer simulations have provided a useful tool for understanding the structure of water on mineral surfaces on the atomistic level. While previous molecular dynamics (MD) studies have revealed the structure of water on 2-dimensional flat surfaces, here we use MD simulations to describe the structure of water around 3-dimensional hematite nanoparticles. We show that the water is ordered into layers, and have begun to evaluate the orientation of water molecules at distinct sites around the surface. We also describe how the change in surface charge can affect not only the order and orientation of water but also the transport of aqueous ions to the surface. By performing MD studies of nanoparticles immersed in solutions of varied ionic strength we investigate how the change in the surface charge gradients affects the structure and distribution of the electrolyte aqueous solution around it. Finally we evaluate how the structure of water can influence aggregation of two or more hematite nanoparticles and suggest a mechanism for aligning nanoparticles during growth via oriented aggregation.