Shedding Light on Peptide Controlled Silica Mineralization

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Biominerals are fascinating composites of organic and inorganic matter that have evolved over hundreds of millions of years. With their intricate nano- to microscale architecture, biominerals display extraordinary properties in terms of toughness, strength and weight. These properties are found for example in the silica cell walls of diatoms. The formation of silica in diatoms has been well-studied on the macroscopic scale. However, the implementation of biomimetic silica formation in technological applications requires a molecular-level understanding of how silica morphology is controlled by organic molecules. Peptides are one class of organic molecules that have been used extensively to mimic biomolecules involved in diatom biosilicification. In this thesis I study how peptide structure and ordering at interfaces influences the morphology of artificially generated silica.

Helical and β-strand artificial amphiphilic peptides mineralize different silica morphologies at the air-water interface. Surprisingly, even minimal changes to these peptides, such as a protecting group, can result in substantially different morphologies. Interrogating natural biosilicification further, a structural investigation of the R5 peptide – a derivative of the diatom peptide Silaffin – is presented. Finally, an approach is presented to benchmark different parameter sets for molecular dynamics simulations of peptides at the air-water interface.