bonds with water than POM, resulting in excellent water solubility. This conclusion was verified experimentally using infrared and dielectric spectroscopies, as well as theoretically using force-field molecular dynamics. In the theoretical study, PEG molecules uniformly mixed with water molecules after 1 ns, while POM chains still aggregated locally within the same time frame. When the oxygen charge density of POM was increased to the value of PEG, POM started to disperse among the water molecules uniformly, meaning its solubility enhanced considerably.

Qigang Wang of Tongji University, China, highlights the significance of this work: "It is tricky to predict the water solubilities of macromolecules, as they do not always obey the 'like dissolves like' principle and empirical rules valid for small molecules. The advanced spectroscopy techniques and the comprehensive molecular simulations demonstrated in this work constitute a novel toolbox to tackle this challenge."

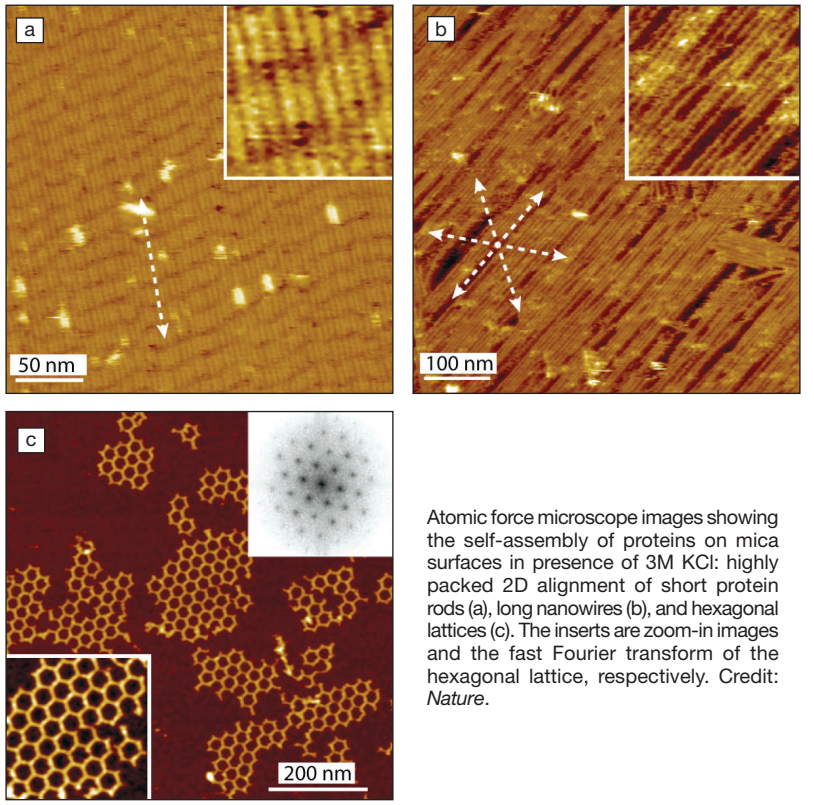
The conclusion reported in this work is also applicable to explain the water solubilities of other polyethers, for example, dioxane versus trioxane. More generally, this work provides a new theory to predict the water solubilities of oxygen-containing polymers.

Tianyu Liu

Proteins designed to bind to a specific surface

Proteins are organic biopolymers consisting of a sequence of smaller amino-acid units. However, unlike synthetic polymers, which are made from a single monomer repeated over and over, these amino acids come from a library of 20 different varieties, enabling proteins to fold into complex three-dimensional (3D) shapes that directly control their function. The research led by James J. De Yoreo and David Baker from the Pacific Northwest National Laboratory and the University of Washington, and published in a recent issue of *Nature* (doi:10.1038/s41586-019-1361-6) focus on the self-assembly of proteins in the presence of crystals. Indeed, from ice-binding proteins to bone formation, there are indications showing that proteins and minerals can show strong binding affinity and play a role in the mineralization process.

To study the binding of proteins to mineral surfaces, the team designed proteins that specifically bind to mica and self-assemble into ordered patterns on this surface. This binding is driven not only by electrostatics, but also via the specific 3D shapes that proteins adopt in liquid, to allow the carboxyl groups on the protein to match the crystal lattice. Therefore, to design the protein, they used a preexisting helical repeat protein (DHR) whose repeat unit is close to the spacing of the target mica lattice, namely 1.04 nm. The main hypothesis that the researchers validated is that for a protein to adsorb in a predictable orientation onto the surface, the carboxylate groups of the protein should be spaced with the same distances as the atoms of the surface.



Atomic force microscope images showing the self-assembly of proteins on mica surfaces in presence of 3M KCl: highly packed 2D alignment of short protein rods (a), long nanowires (b), and hexagonal lattices (c). The inserts are zoom-in images and the fast Fourier transform of the hexagonal lattice, respectively. Credit: *Nature*.

First, the researchers used simulation tools to predict which protein sequence with the DHR repeat unit is required to achieve this specific binding. This sequence was then used to modify the DNA of a bacteria that was cultured to produce the artificially designed protein *in vivo*. After separation and purification of the protein, they used atomic force microscopy (AFM) to visualize the self-assembled protein structures onto mica. In a typical experiment, the protein solution was deposited onto the mica surface in the presence of K^+ ions. These ions play an important role in defining the interactions between the protein and the surface, which in turn impacts their assembly into designed structures. Scanning the surface with AFM, they observed the formation of liquid-crystal-like assemblies that depended on the ion concentration and the protein sequence. By incorporating protein–protein interactions, they could design, model, and

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fabricate various kinds of assemblies, including coaligned single protein nanowires and hexagonal lattices (see Figure).

Akshita Kumar Dhawan, a postdoctoral researcher at the Centre for Biomimetic Sensor Science at the Nanyang Technological University in Singapore who did not participate in the study, comments that it is "an impressive demonstration of conceiving such degree of control over structured protein–mineral interfaces at various length scales, and the possibility to tailor design them. This is certainly a milestone study that opens multiple avenues in materials and structural biology research." She adds, "Although an intriguing question is the role of water and salts in the packing of the proteins on the surface." Actually, Harley Pyles and Shuai Zhang, the first authors of the study, explain that this is the focus of a future manuscript currently under preparation.

With this work, De Yoreo, Baker, Pyles and Zhang, the four authors, dream "to achieve the same capability of control as found in bones but for functional materials such as semiconductors and photovoltaics, including the ability to drive the morphogenesis of multiple types, such as *p*- and *n*-types or acceptors and donors." Baker says, "Being able to design such systems *de novo* may enable self-assembling architectures of such materials at high packing density in 3D."

Hortense Le Ferrand

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