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John Suske/EyeEm/Getty Image

FILTRATION MEMBRANES

The silk road

The integration of simulations and experiments enable the production of layered water purification membranes with improved performance, report Markus Buehler and colleagues in *Science Advances*.

Membranes that efficiently block molecular-level contaminants are important for mitigating the problem of water pollution. The ideal membrane, apart from having good purification performance, is cheap and mechanically strong. The use of a multilayered architecture can be advantageous, because it endows membranes with high throughput, filter efficiency and molecular loading capacity. However, achieving multilayered structures is complex and time consuming, and the resulting mechanical properties are often far from excellent. Biomaterials are particularly attractive for water purification membranes because they are low cost, environmentally friendly and biocompatible, but so far only membranes with small and non-tunable pore sizes have been reported. The realization of multilayered, biomaterial-based membranes is thus desirable but challenging, because it requires a deep understanding of the molecular and chemical interactions involved.

The researchers used computer simulations to optimize the elements constituting the membranes. “We wanted to explore novel silk-based materials and the use of structural hierarchy in these proteins to generate new functional materials by the ‘universality–diversity paradigm’, creating functionally complex materials out of simple building blocks,” explains Buehler. The idea is to combine a soft and hard material: silk nanofibrils and a calcium-based mineral. The soft component has smaller pores, which ensures size selectivity and efficient filtration of molecular-level contaminants. The hard component has larger pores that allow water to flow quickly through the layer; its rigidity provides structural support to the membrane. The simulations show that the two materials can form either multilayered structures or homogeneous mixtures. By varying the parameters of these materials, in particular the density and stiffness, the researchers can elucidate how the interfacial energy governs the assembly. To obtain a layered structure, the interaction between the protein nanofibrils and the minerals has to be weaker than the protein–protein and mineral–mineral interactions. The insight gained from the simulations is used to select the combination of materials best suited for the fabrication of a layered structure.

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To produce the layered material, the silk nanofibrils are first self-assembled in water and are then used as templates for the growth of mineral nanocrystals by *in situ* biomineralization. The membrane is finally formed by removing the liquid through vacuum filtration. The volume of the dispersion determines the thickness of the membrane and the number of layers; membranes with tens of alternating layers can be obtained. The resulting membranes exhibit good mechanical flexibility and toughness, which is important for durability. The membranes can also be formed directly on the filter of commercial syringes, producing low-cost syringe ultrafilters. The performance of the membranes in terms of water flux and separation of proteins, colloids and dyes is very good. In addition, they can absorb heavy metal ions, which are toxic and difficult to remove (these ions are usually smaller than the pore sizes). The toxic ions can then be removed and safely recycled. “In the long run, these biodegradable, green and simple membranes may provide an option for the generation of cleaner water in developing countries where infrastructure may be lacking,” says Buehler.

The membranes presented in this work are attractive because of the combination of rapid fabrication, low cost and good performance. Future goals include “generating larger biomimetic multilayered membranes with high filtration capability, enhancing the selectivity for chemical separation and optimizing membrane recovery and reuse,” concludes Buehler. Computer simulations can be used to predict other promising combinations of materials, which could include engineered proteins — this strategy will enable the efficient design of membranes with controllable properties.

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ORIGINAL ARTICLE Ling, S. *et al.* Design and function of biomimetic multilayer water purification membranes. *Sci. Adv.* **3**, e1601939 (2017)