Researchers discover new shapes of microcompartments

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In nature and engineering, microcompartments — molecular shells made of proteins that can encapsulate cellular components — provide a tiny home for important reactions. In bacterial organelles, for example, microcompartments known as carboxysomes trap carbon dioxide and convert it into sugar as an energy source.

These shells naturally buckle into a specialized 20-sided shape called an icosahedron. But now researchers at Northwestern University's McCormick School of Engineering and Applied Science have discovered and explored new shapes of microcompartment shells. Understanding just how these shells form could lead to designed microreactors that mimic the functions of these cell containers or deliver therapeutic materials to cells at specific targeted locations.

The research, led by Monica Olvera de la Cruz, professor of materials science and chemical and biological engineering and chemistry, with Graziano Vernizzi, research assistant professor, and research associate Rastko Sknepnek, was recently published in the Proceedings of the National Academy of Sciences.

Olvera de la Cruz and her group knew how shells made up of just one structural unit worked — their elasticity and rigidity cause them to naturally buckle into icosahedra. But they began considering how to create heterogenous shells by using more than one component. Using physical concepts, mathematical analysis, and running simulations, they formulated a new model for the spontaneous faceting of shells.

"The question was: if a shell is made up of components that have different rigidities or different mechanical properties, what would be the shape it takes?" Olvera de la Cruz said.

The only faceted shape previously known for molecular closed shells, such as viruses and fullerenes, was the icosahedron. But Olvera de la Cruz and her colleagues discovered that when a shell is made up of two components with different elasticities, they buckle into many different shapes, including dodecahedra (12 sides) and octahedra (8 sides) and irregular polyhedra, which surfaces are "decorated" by the natural segregation of components to yield the lowest energy conformation.

Some of these shapes had been seen in nature before — sometimes in the bacterial organelles' carboxysomes — but they were just called "quasi-icosahedra" because nobody knew how to characterize them and how they worked. Armed with their model, however, engineers could now potentially design shells to perform specific tasks.

"If you just want to pack something into a shell, you use a sphere," she said. "But if you want to create a shell that has intelligence and can fit somewhere perfectly because it is decorated with the right proteins, then you can use different shapes."

These designed shells could act as containers or microreactors within the body. "It's a very efficient way to deliver something," she said.

Next the group hopes to determine how general their model is and continue researching how different shapes are made.

"I think it can open a new field of research," Olvera de la Cruz said.

Provided by Northwestern University