Chemists 'crystallize' new approach to materials science

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A team of chemists at the University of California San Diego conducted breakthrough research for materials science—a field for which chemistry frequently provides information about the structure and composition of materials, as well as the processes for making and using them. Its aim is to create new materials—from metals and rubber to coatings and crystals.

Researchers in the Department of Chemistry and Biochemistry accomplished this goal by mixing together unlikely materials to create a new hybrid form of crystalline matter that could change the practice of materials science. The findings, published in *Nature*, present potential benefits to medicine and the pharmaceutical industry.

Ling Zhang, Jake Bailey and Rohit Subramanian, all Ph.D. candidates studying under Professor Akif Tezcan, combined protein crystals with synthetic polymers to create the new hybrid materials.

"The chemical integration of two such disparate substances gives rise to a new form of matter that completely circumvents the fundamental limitation that ordered substances are brittle and inflexible, and flexible materials are devoid of order," explained Tezcan, who operates Tezcan Lab at UC San Diego.

Crystals are arrays of atoms or molecules periodically ordered in three-dimensional space through specific interactions. Because these interactions hold the neighboring constituents in a unique arrangement, crystals—like grains of salt, for example—cannot flex or expand. Instead, if hit by a blunt force, they shatter into pieces which cannot rejoin. The researchers circumvented these fundamental limitations by infusing protein crystals with a network of hydrogel polymers, which are essentially floppy, sticky chains that form a shape-memory mold around the protein molecules. This mold enables the protein crystals to heal themselves when they crack, as well as to expand (sometimes by up to 500 percent in volume) and contract without losing their crystallinity. In fact, the UC San Diego researchers observed that in some instances the atomic-level order of the protein molecules increased upon expansion and contraction. The increased order enabled the researchers to use X-ray radiation to obtain higher-resolution structures than ever observed for a protein called ferritin (produced in a variety of organisms to store iron).

According to Tezcan, these results offer promise for using the strategy generally to improve the X-ray crystallography of proteins, the pre-dominant method to examine the atomic structures and functions. The crystal-hydrogel hybrids also provide a blueprint for making simultaneously tough and strong materials that can withstand fracture. What's more, the ability of these materials to expand and contract may perhaps be used to safely store large biological agents like antibodies and nucleic acids, and then to release them in desired locations in the body for therapeutic purposes.

"These materials uniquely combine the structural order and periodicity of molecular crystals, the adaptiveness and tunable mechanical properties of synthetic polymers, and the chemical versatility of protein building blocks," said Tezcan. "The most enjoyable part about this work was how it combined different disciplines and techniques in unforeseen ways to create new research directions."

More information: Ling Zhang et al. Hyperexpandable, self-healing

macromolecular crystals with integrated polymer networks, *Nature* (2018). DOI: 10.1038/s41586-018-0057-7

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