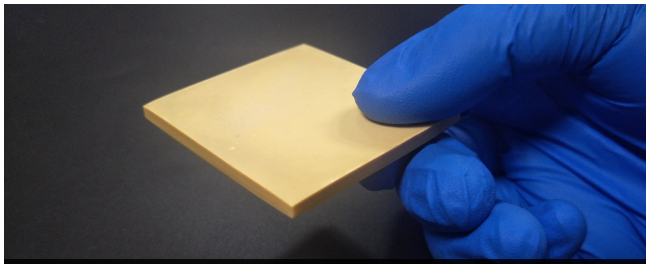
Mimicking nature's toughest materials

Research is firming up around the commercial production of BIOMIMETIC MOTHER-OF-PEARL.



Complex composites inspired by ultra-tough shell are close to commercial sizes.

It hasn't slipped past material scientists that some of nature's strongest materials, including bone and nacre/mother-of-pearl, are composed of layers of nanosized mineral platelets bonded by a flexible biopolymer matrix. But the complexity of these hierarchically ordered structures has made biomimetic production too expensive.

In 2020, in *Nature Communications*, a team led by Shu-Hong Yu detailed the rapid bulk-production of low-cost eco-friendly mimetic-nacre using a unidirectional pressing technique, cellulose nanofibers and mica micro-platelets. The material demonstrates better strength and thermal stability than petroleum-based plastics.

"We focused on the often overlooked processes of how organisms create these natural materials," explains Yu. This approach was also behind a mineralization technique reported by the team in 2016 in *Science*. The method featured aragonite nanocrystals reminiscent of nacre's aragonite platelets precipitated from a solution containing calcium bicarbonate, similar to the secretions of nacre-lined molluscs.

In 2017, the team used water-evaporation-aided lamination to form large nacre-mimetic composites of greater thickness.

"Ultimately, we would like to engineer more sustainable materials, and to also contribute to fields including tissue engineering and aerospace," Yu says. His team are also investigating the twisted, layered structures found in the armour of some insects, and the unidirectionally porous structure of natural wood. ■

HPC software for powerful quantum chemistry simulations

New supercomputing code is enabling LARGE-SCALE ATOMIC-LEVEL QUANTUM CHEMISTRY SIMULATIONS for the first time.

Sunway TaihuLight is simulating quantum chemistry reactions at unseen scales.

Researchers led by Jin-Long Yang are developing code that is moving the scope of precise atomic-level quantum chemistry simulations up to a few hundred thousand atoms, making it possible to simulate bulk material quantum dynamics with atomic precision for the first time.

"We are applying high-performance computing to quantum chemistry with the goal of realizing large-scale and high-precision first-principles calculations," says Yang, head of the Division of Theoretical and Computational Science.

Using Sunway TaihuLight, a supercomputer with 10 million Chinese-designed processors and a unique master-slave processor architecture for high internal parallelization, the team has developed its own code for efficiently running quantum chemistry algorithms and simulating chemical reaction phenomena at previously unseen scales.

"High-precision quantum chemistry and materials science simulations on other platforms and software have so far been limited to thousands of atoms," says lead code developer, Wei Hu. "To simulate systems of hundreds of thousands of atoms and their quantum interactions, we need new code that can use as many parallel processor cores as possible."

These new code packages are now available to any researcher and can simulate a large system of thousands of atoms in just 10 minutes. Such previously unattainable simulations represent a tremendous boost in the search and design of new functional materials. ■

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