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New hybrid molecules could lead to materials that function at the nanoscale

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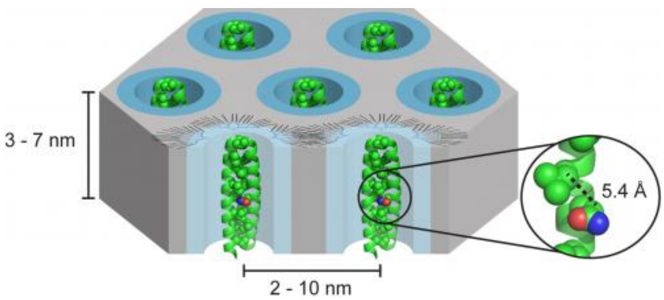

The outcome of the CAREER Award will be new materials with predictable structure and organication on both the molecular scale and nanoscale. A new molecular architecture, dendornized helix bundle assemblies, will be developed under this award. The new molecules are hybrids of highly branched polymers called dendrons, which promote organization of the 2-D hexagonal array structure having dimensions ~2-10nm, and helical peptides that associate into protein-like bundles. The bundles have a discrete height (~7-10nm), and the precise arrangement of atoms in the bundle can be used to create functional materials such as selectively permeable membranes. Credit: Jonathan G. Rudick, Stony Brook University

Synthetic chemists today have the ability to construct molecules of almost any atomic composition, creating new materials with any number of promising applications that range from sustainable energy and environmental remediation, to high-performance electronics.

"It is possible to finely tune the properties of molecules through chemical synthesis to achieve just the right balance of properties needed," says Jonathan Rudick, an assistant professor of chemistry at Stony Brook University. "For example, through chemical synthesis, we can select ranges of the solar spectrum that a molecule will absorb, which has been essential for progress made in the area of organic molecules for solar power."

The National Science Foundation (NSF)-funded scientist is studying a class of molecules known as dendrons, highly branched molecules shaped like wedges or cones, which pack together to form circular or spherical assemblies with nanoscale dimensions. His group aims to develop a new class of nanoscale materials that can be processed like conventional synthetic polymers, yet retain the high structured order found in proteins.

One potential benefit of their work could be in developing a low-cost, low-weight and compact material that could be used to purify large volumes of water, and prove valuable in developing countries where potable water is difficult to find. It also could be useful in large scale water treatment facilities "where you need to be able to purify large volumes quickly, and the less membrane it takes to do that, the better," he says.

This requires creating the tiniest of channels for the water to pass through, which is not as simple as it sounds.

"The composition lining of the hole determines whether the water will go through," he says. "When you get a hole down to being the size of a molecule, then the interactions between the atoms in the water molecule and the atoms that line the hole become critical as to whether or not the water will go through. It's not like shooting water through a faucet."

Dendrons pose a special challenge in that "there is very little order to how the atoms are arranged within their assembly," making it difficult for scientists to manipulate the atoms, Rudick says.

However, peptides, on the other hand, another class of molecules "can take on a helical conformation, in which the atoms are arranged like a spiral staircase," with known locations for each atom, he explains. "Because the location of each atom in the helical molecule is known, we can accurately anticipate the positions of atoms in bundles of helical peptides."

Their approach, then, is to attempt to design a hybrid using the best features of each. The result would be a new class of molecules, dendronized helix bundle assemblies.

"We anticipate that this new class of materials will allow us to more accurately understand how materials function at the nanoscale," he says.

"We are trying to prove the concept that we can create a material where you can have atomic level control," he adds. "We synthesize new materials. We make these new materials, and we are characterizing the structure of films that can be made from them."

Dendronized helix bundle assemblies "represents a class of molecules that has never been made before," he says. "It's a class of polymer with a perfectly branched molecular structure. We refer to them as 'bio hybrid molecules,' because part is something found in nature, and the other part is synthetic. We are covalently attaching sequences of amino acids that might be found in helical proteins in nature to dendrons."

He is conducting his research under a NSF Faculty Early Career Development (CAREER) award. The grant supports junior faculty who exemplify the role of teacher-scholars through outstanding research, excellent education, and the integration of education and research within the context of the mission of their organization. NSF is funding his work with about $500,000 over five years.

As part of the grant's educational component, his lab is working with a local high school to teach students about liquid crystals and other forms of soft matter.

Dendronized helix bundle assemblies also could have a major impact in the development of molecular materials for solar power, he says.

"The active components in organic photovoltaic materials are organic molecules that can absorb light called chromophores," he explains. "The arrangement of chromophores in a film plays an important role in determining whether an absorbed photon of light is transformed into energy we can use.

"Furthermore, the best arrangement of chromophores is not yet known, and will likely vary depending on the particular chromophore being used," he adds. "By incorporating chromophores within the helical bundle portion of our hybrid molecular materials, we will be able to systematically explore how to optimize the performance of solar conversion materials."

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