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IMITATING NATURE: SELF-ASSEMBLY TECHNIQUE MAY BUILD DESIGNER POLYMERS FROM MODULAR SCAFFOLDS & BUILDING BLOCKS

Future designer polymers may be assembled like children's Lego toys using modular polymer scaffolds programmed to attract building blocks of small molecules. Weak and easily reversed chemical interactions would self-assemble those molecules to form complex structures with predictable physical and chemical properties.

In the natural world, self-assembly techniques produce thousands of varied life forms -- bacteria to human beings -- based on a relatively small set of amino acids and nucleosides combined in different ways. By emulating this natural system, polymer chemists at the Georgia Institute of Technology hope to simplify the synthesis of new materials for light-emitting diodes, optical storage materials, biosensors, drug-delivery materials and other applications.

Already, the researchers have built copolymers that use independent chemical bonding mechanisms -- also copied from the biological world -- to simultaneously self-assemble two building-block functional groups through a simple "one-beaker" process.

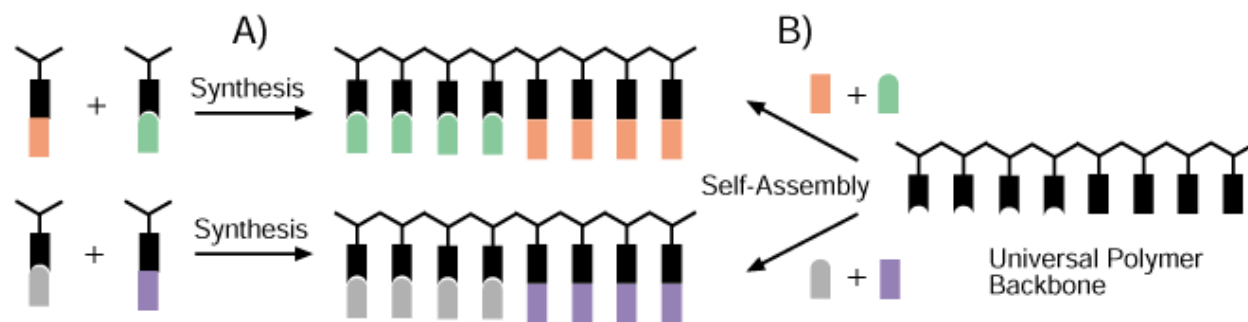
"The goal is to simplify the synthesis of designer polymers via self-assembly using

combinatorial chemistry," said Marcus Weck, assistant professor in Georgia Tech's School of Chemistry and Biochemistry. "Our group is taking design lessons from Nature by incorporating into one system several of these weak interactions to get a degree of complexity that is difficult to achieve otherwise. We believe we now have the basic proof of principle to show that we will be able to address this problem."

He explained the concept and described research progress August 18th at the 224th national meeting of the American Chemical Society in Boston.

"We are developing a system based on a polymer that contains two or three different basic units, each having a different recognition motive for weak interactions," Weck explained. "We would ultimately want to have a shelf with 30 or 40 polymer backbones. When someone needed a new LED, for instance, we would just take our polymer backbones, synthesize small molecules, then self-assemble them onto the polymer backbones. In one simple step in a beaker on the lab bench, we could assemble the polymer instead of taking two or three months to synthesize it with traditional methods."

Using a multi-step self-assembly process based on weak hydrogen bonding or metal coordination, Weck and his colleagues build --



Comparison of the strategies to obtain copolymers: (A) traditional "living" polymerization strategy and (B) the self-assembly strategy. Conventional strategy (A) relies on the living polymerization of monomers, while the self-assembly method is based on a universal backbone and the controlled self-assembly of side-chains onto the backbone.

and sometimes take apart -- complex structures based on their polymer backbones. By changing such variables as temperature, pH, ultraviolet light and solvent, the researchers add and subtract the small functional groups that give the structure its final properties.

Weck envisions a system of polymer scaffolds, each with slightly different mechanical properties, such as strength, flexibility and hardness. Each scaffold would have bonding sites engineered to attract specific small molecules found in a collection of such functional structures. Placing the scaffolds into a chemical bath containing one or more of these functional molecules would initiate a self-assembly process that would add those small molecules to the structure. Multiple steps could build complex structures with the desired electronic, biological or optical properties.

With thousands of combinations possible, the process could quickly produce new materials for testing by engineers seeking new materials with specific properties. If those prototype materials failed to meet the need, reversing a chemical bond would allow one of the small molecules to be removed and replaced with an alternative for further study. Weck compares that to the "plug-and-play" system used to connect computer peripherals.

"We could eliminate the elongated and complicated synthesis of polymers and go directly to something that has the strength we want, but is reversible," he said. "We hope that our system will reduce the time required to synthesize and test new chemical structures."

The researchers -- including Joel M. Pollino, Ludger P. Stubbs, Amy Meyers, Joseph Carlise and Robert Kriegel -- have so far used hydrogen bonding and metal coordination bonding together in a structure able to self-assemble different molecules using the two independent bonding methods. In preliminary testing, the different techniques appear compatible, with a molecule being joined to one bonding system not affecting a molecule already joined using the other system.

Potential chemical interference problems pose the greatest technological hurdle to the new system, Weck notes. To build up complex structures using self-assembly processes, he must be able to insert new molecules without affecting molecules already part of the structure or disabling other bonding systems. Natural systems do that well, but synthetic chemical processes often suffer from unintended interactions.

"We have found some very nice systems that have very good properties and will self-assemble and recognize our system very easily," he said. "We now have a polymer backbone that has metal coordination sites and hydrogen bonding sites. That means we can now add two small molecules at a time. Each small molecule is programmed to fit its place on the backbone, where it self-assembles and give us a new material."

The approach varies the strength of chemical interactions to gain the right properties. In drug delivery systems, for instance, weak interactions may be used to allow a therapeutic molecule to easily drop off the polymer deliver molecule at the proper location in the body. But molecules used in light-emitting diodes would require stronger bonds to hold the structures together for the expected operating life of the device.

Because of the cost and complexity, Weck's system would likely be used only for expensive specialty applications. Current commodity polymer uses would continue to be produced using traditional polymerization techniques, he said.

Weck's group has published papers on their approach in the journals *Synthesis* and *Organic Letters*. The research has been sponsored by the Petroleum Research Fund of the American Chemical Society and by a grant from the 3M Corporation.

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