

Reproducing nature's chemistry: Researchers alter molecular properties in a new way

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New technique alters molecules' environment to obtain specific properties

In their search for molecules with certain characteristics, chemists have produced millions of new, increasingly complex synthetic materials by altering molecules' chemical structures.

Taking cues from nature, Northwestern University researchers have recently tested a new method for achieving the molecular properties they seek: by changing the geometry of the surface to which molecules are bound.

"For years chemists have been making molecules to solve problems — each one more synthetically complicated than the last — but we still haven't come close to achieving what nature can do with much simpler chemistry," said Bartosz A. Grzybowski, Kenneth Burgess Professor of Chemical and Biological Engineering and Chemistry at Northwestern's McCormick School of Engineering and Applied Science. "Nature's most complex component of life, the protein, is made from only 21 simple amino acids. This research explores the idea that it's not the molecule you have that's important, it is how it interacts with its environment."

Using this idea, the researchers developed a technique in which a single type of molecule is placed on nanoparticles with two different regions of curvature. Although the molecules are atomically identical, they demonstrate unique chemical properties depending on what region of curvature they are bound to.

A paper describing the research, "Geometric Curvature Controls the Chemical Patchiness and Self-Assembly of Nanoparticles," was published August 18 in *Nature Nanotechnology*.

The researchers began by affixing molecules of a carboxylic acid at various points on several gold nanoparticles, some as small as five nanometers in diameter. Each nanoparticle possessed a different geometry. On nanoparticles exhibiting a greater curvature, the molecules were naturally spaced farther apart; on nanoparticles with more gradual curvature, they were closer together.

The differences in curvature influences the distance between the molecules, making it possible for the researchers to induce so-called "patchiness" on cylindrical- and dumbbell-shaped nanoparticles. Essentially, the molecules can "feel" each other through repulsive electrostatic interactions and, as the carboxylic acids are deprotonated, the difficulty in adding more charges onto the nanoparticles is controlled by how crowded the molecules are. These "patchy" nanoparticles can interact and self-assemble directionally, mimicking chemical molecular bonds —

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and, the researchers found, altering when the charge of these attached molecules changes.

"Changing molecular properties by altering environments instead of molecular structure could free scientists to accomplish more with a smaller library of already existing molecules, and could offer alternatives to chemical processes that often require toxic chemicals," said David Walker, a graduate student in McCormick's Department of Chemical and Biological Engineering and the paper's first author.

The curvature phenomenon is specific to the nano-scale, where most of the chemistry in biological systems is performed, and begins to fail for nanoparticles above 10 nanometers in diameter, the researchers said. "Larger particles have curvatures that are just too subtle for the molecules to feel the effect — similar to how humans might perceive the Earth to be flat, even though we now know better," Walker said.

The researchers are currently working to extend the work to other classes of molecules that could be beneficial for catalysis and energy purposes.

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