Researchers' work in catalysis could aid drug development

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Many molecules have a chemical structure that is "chiral" - they come in two forms, each with an arrangement of atoms that are mirror images of each other.

These "right-handed" and "left-handed" arrangements, called enantiomers, are problematic for industries that make pharmaceuticals and agrochemicals.

Proteins and sugars in the human body exist in only one of the two enantiomers. Yet the catalytic reactions involved in making drugs often produce molecules with both the "right-handed" and "left-handed" arrangements.

"The handedness of molecules that we ingest, such as drugs, can behave differently depending on whether they are left- or right-handed, often with catastrophic consequences," says Wilfred Tysoe, UWM distinguished professor of chemistry and biochemistry.

That means that drugs have to be synthesized to have only one "handedness." Current chiral catalysts that can accomplish this task mix tightly with the reactants, making them difficult to separate afterwards.

The goal is to develop a solid "chiral" catalyst that can easily be separated from its products.

New research from the Tysoe group at the University of Wisconsin-

Milwaukee helps to bring that goal closer to reality. The researchers uncovered what happens on the surface of a solid chiral catalyst that allows the preferential formation of only one enantiomer of a molecule.

The work, funded by the U.S. Department of Energy, is detailed in a paper published today in the journal *Nature Communications*.

The work was carried out in collaboration with Dilano Saldin, a UWM distinguished professor of physics; post-doctoral researchers Mausumi Mahapatra, Michael Garvey and Yun Bai; and chemistry graduate student Luke Burkholder.

The researchers put a chiral molecule on the surface of a heterogeneous catalyst to investigate how the catalyst biased the surface to favor a particular handedness.

"A major problem with designing such catalysts arises from the fact that it is difficult to completely influence all of the places on the extended metal surface where the reaction takes place," said Tysoe. "So any unmodified positions on the surface will produce both right- and left-handed molecules."

Rather than using a complex commercial catalyst, the team used a simplified catalyst that retained the commercial version's key chemical properties. This allowed them to use a Scanning Tunneling Microscope to "see" which molecules adsorb and interact on the catalyst surface.

"We found that the reactant molecules undergo a structural change when it interacts with the chiral modifier which leads to the preferential formation of one enantiomer, and also makes it more reactive," Tysoe said.

Provided by University of Wisconsin - Milwaukee

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