Novel method of squeezing molecules together could reduce chemical manufacturing waste

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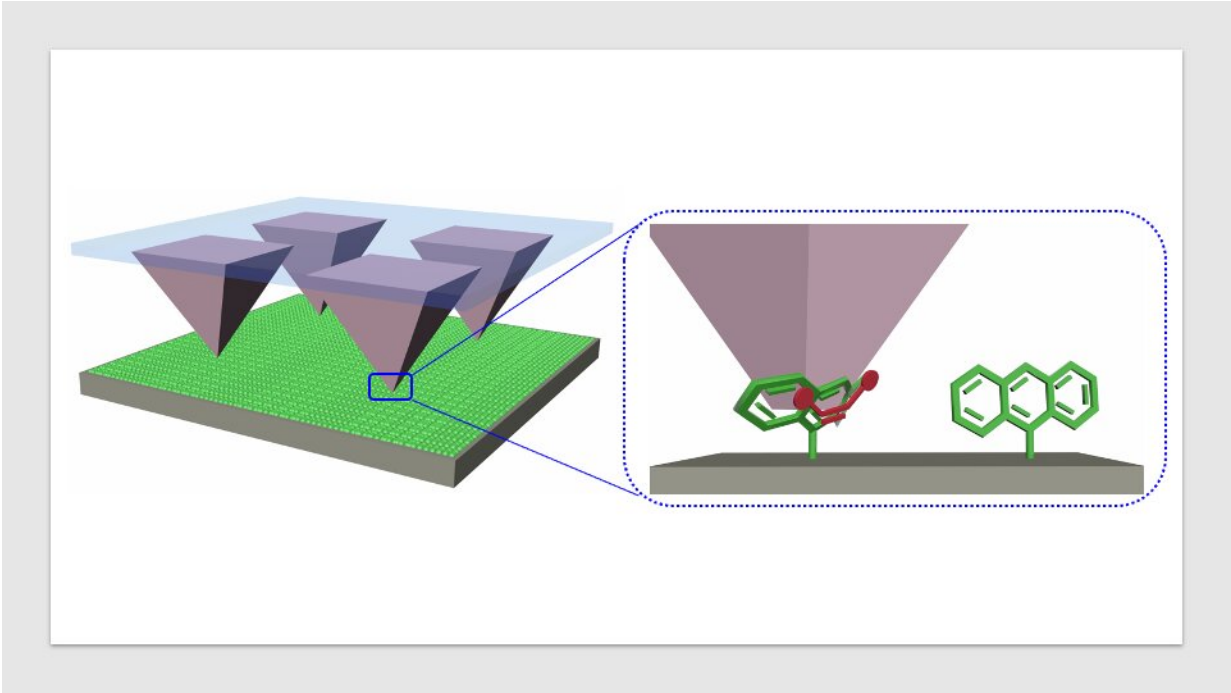

Tip arrays transfer a dienophile molecules (red) onto an anthracene-modified (green) surface. Upon contact, the tips form nanoreactors, where pressure is applied that accelerates the Diels-Alder cycloaddition reactions. For their study, the authors took monolayers of molecules placed on silicon wafers and pushed reactive molecules into them using tip arrays, which created new chemicals. The experimental setup allowed the researchers to precisely control the pressure between the molecules, which led to a new understanding of what occurs in these reactions. Credit: Yerzhan Zholdassov

The production of chemicals accounts for 40% of all energy currently used in manufacturing, and the process also results in toxic solvent waste that pollutes the environment and poses health risks to humans and animals. A study published in the journal *Science* details a novel mechanochemistry method that has the ability to manufacture chemicals without those deleterious effects.

Researchers with the Nanoscience Initiative at the Advanced Science Research Center at the CUNY Graduate Center (CUNY ASRC), the University of Pennsylvania, and the University of California-Merced took a unique approach that advances the opportunity to use mechanochemistry in large-scale production. The technique uses organic chemistry and nanotechnology to push molecules together and create chemicals without the use of costly solvents that pollute the environment. The research team's findings have major implications for numerous manufacturing sectors, including the production of pharmaceuticals and materials for a variety of medical and industrial purposes.

"This is a really exciting breakthrough, because the discovery makes mechanochemistry a reliable means of producing chemicals, and it allows us to do so without the harmful byproducts and large energy demands of current manufacturing techniques," said the study's lead author Adam Braunschweig, a professor of Chemistry and Biochemistry with the CUNY ASRC Nanoscience Initiative and Hunter College Department of Chemistry.

"When we pushed on the molecules, we found that they twisted into new, more reactive shapes that require less energy to combine and produce a desired chemical," said first author Yerzhan Zholdassov, a doctoral student with the Braunschweig Lab.

The experiment allowed researchers to measure the amount of force needed to create a predictable and reliable chemical reaction and show

that mechanochemistry is a viable and scalable technique for manufacturing chemicals in a more sustainable, cost-efficient manner. The new technique can also be used to create new drugs and materials that can't be created using current techniques that rely on solvents.

Co-author Robert Carpick, a professor in the University of Pennsylvania's Department of Mechanical Engineering and Applied Mechanics who collaborated on this project, added, "This discovery was not possible without chemists teaming up with mechanical engineers in a truly cross-disciplinary way. The chemists were critical to designing and conducting the experiments, but we had to combine their forefront chemistry knowledge with advanced mechanics analysis to understand—through experiments and theory—how mechanical forces are accelerating chemical reactions here. The teamwork made the difference."

More information: Yerzhan S. Zholdassov et al, Acceleration of Diels-Alder reactions by mechanical distortion, *Science* (2023). DOI: 10.1126/science.adf5273.
www.science.org/doi/10.1126/science.adf5273

Perspective: Paul S. Weiss, A push for mechanochemistry, *Science* (2023). DOI: 10.1126/science.adi3388.
www.science.org/doi/10.1126/science.adi3388

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