Researchers find promising nanoparticle candidates for carbon dioxide capture and conversion

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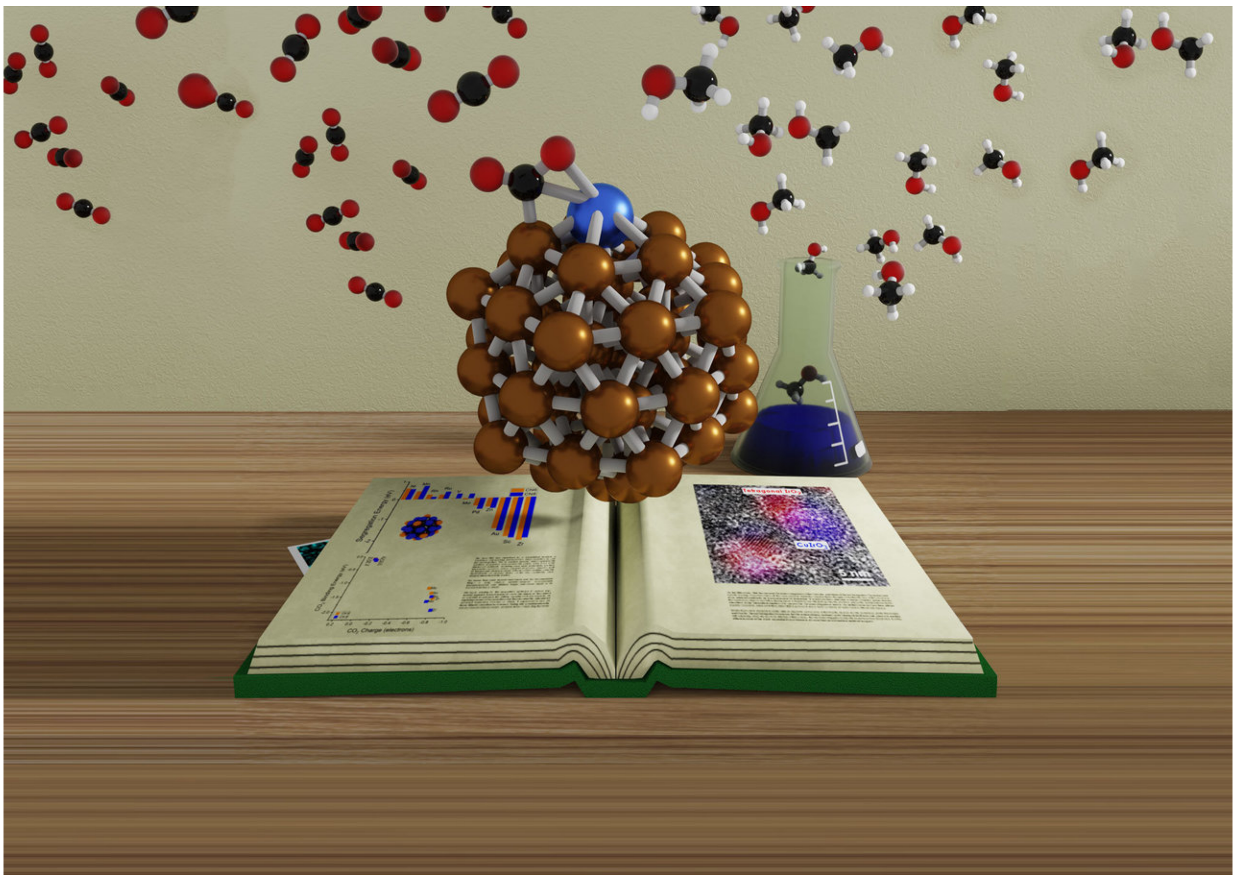

Original artwork from the University of Pittsburgh depicting a copper-based bimetallic nanoparticle designed to adsorb and activate carbon dioxide appeared on the cover of ChemSusChem in April 2018. Credit: Swanson School of Engineering/James Dean

A recent article in the sustainable chemistry journal *ChemSusChem* revealed researchers at the University of Pittsburgh are "doping" nanoparticles to enhance their ability to capture carbon dioxide and provide a raw source of carbon for industrial processes. Not to be confused with its negative use in athletics, "doping" in chemical engineering refers to adding a substance into another material to improve its performance.

Along with global temperatures, research into the capture of carbon dioxide (CO_2) is on the rise. The amount of CO_2 in the atmosphere has reached a historic high of 408 parts per million, according to the latest measurements by NASA. Previous studies have shown the connection between greenhouse gases like CO_2 and the warming trend, which began around the turn of the 20th century.

"Many of our

industrial processes contribute to the alarming amount of CO_2 in the atmosphere, so we need to develop new technologies to intervene," says Giannis Mpourmpakis, assistant professor of chemical and petroleum engineering at Pitt's Swanson School of Engineering. "Capturing CO_2 from the atmosphere and converting it to useful chemicals can be both environmentally and industrially beneficial."

Dr. Mpourmpakis co-authored the study titled "Design of Copper-Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation" in *ChemSusChem*, with other researchers in Pitt's Department of Chemical and Petroleum Engineering including Professor Götz Veserand three Ph.D. students: James Dean, Natalie Austin, and Yahui Yang. An artistic depiction of the zirconium-doped copper nanomaterials appeared on one of the journal's covers for Volume 11, Issue 7 in April 2018.

Through a series of computer simulations and lab experiments, the researchers designed and developed a stable catalyst for the capture and activation of $CO_2$by doping copper nanoparticles with zirconium. The researchers believe the nanoparticles have large potential for reducing the carbon footprint of certain processes such as burning fossil fuels. However, CO_2 molecules are rather reluctant to change.

"CO_2 is a very stable molecule which needs to be 'activated' to convert it. This activation happens by binding CO_2 to catalyst sites that make the carbon-oxygen bond less stable. Our experiments confirmed the computational chemistry calculations in the Mpourmpakis group that doping copper with zirconium creates a good candidate for weakening the CO_2 bonds," explains Dr. Veser.

Mpourmpakis' group used computational chemistry to simulate hundreds of potential experiments vastly more quickly and less expensively than traditional lab methods and identified the most promising candidate dopant which was then experimentally verified.

Copper nanoparticles are well-suited for the conversion of CO_2 to useful chemicals because they are cheap, and they are excellent hydrogenation catalysts. Through hydrogenation, CO_2 can be converted to higher-value chemicals such as methanol (CH_3OH) or methane (CH_4). Unfortunately, converting CO_2 also requires its activation which copper is not able to deliver. Zirconium gets along well with copper and naturally activates CO_2.

"To have an effective dopant, you need to have sites on the catalyst surface that pass electrons to CO_2," says Dr. Mpourmpakis. "The dopant changes the electronic characteristics of materials, and we found zirconium is particularly effective at activating the CO_2."

The Pitt researchers tested a number of different nanoparticle configurations and found the zirconium-doped copper nanoparticles particularly promising catalysts for hydrogenating CO_2 and have already begun testing their effectiveness.

More information: James Dean et al. Design of Copper-Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation, *ChemSusChem* (2018). DOI: 10.1002/cssc.201702342

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