Taming defects in nanoporous materials to put them to a good use

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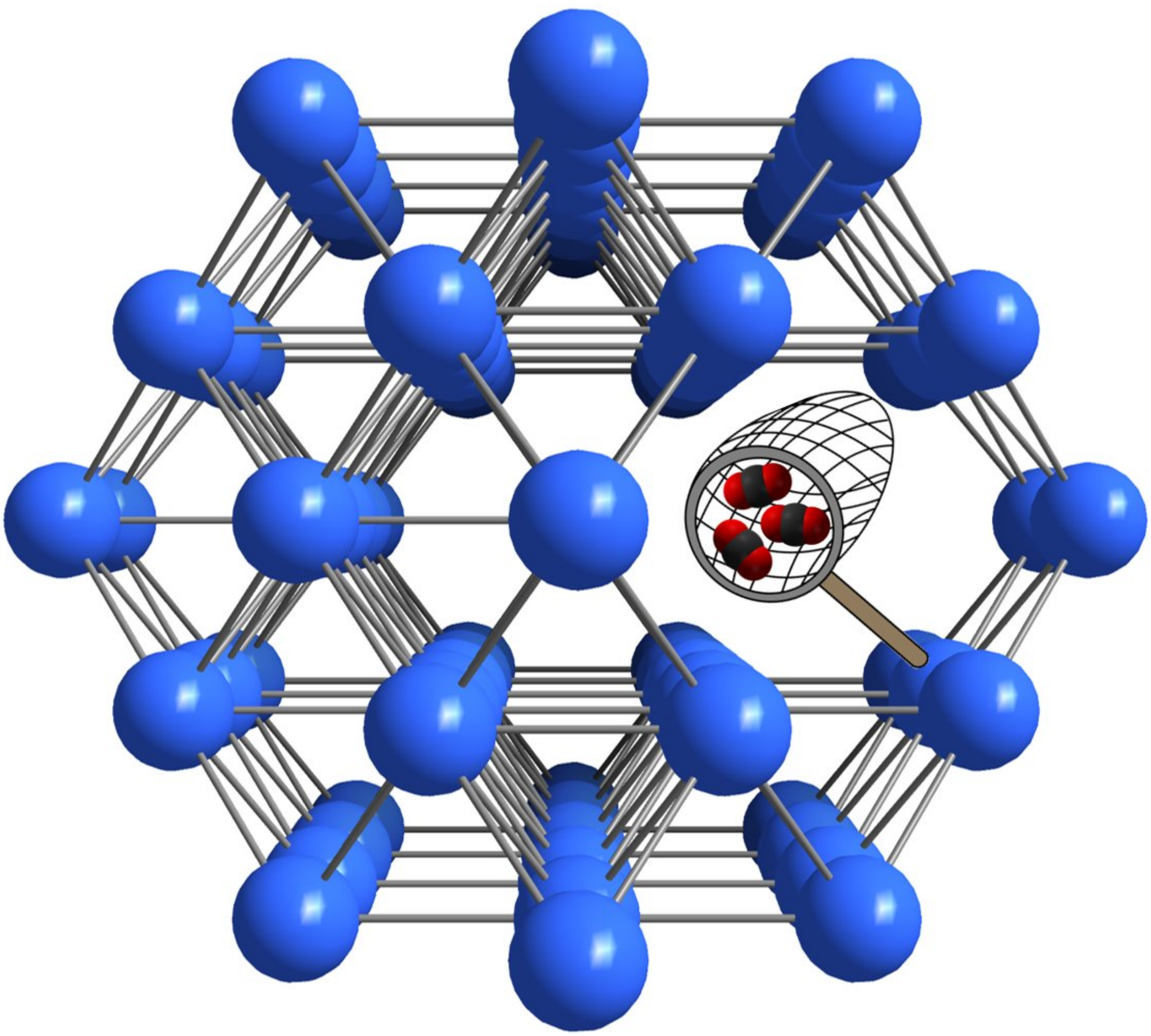

Modification of defective nanoporous materials has unique effects on their properties. Swansea University scientists are seeking to master this method to make new materials to capture CO_2. Credit: Swansea University

The word "defect" universally evokes some negative, undesirable feature, but researchers at the Energy Safety Research Institute (ESRI) at Swansea University have a different opinion: in the realm of nanoporous materials, defects can be put to a good use, if one knows how to tame them.

Metal Organic Frameworks

A team led by Dr. Marco Taddei, Marie Sklodowska-Curie Actions Fellow at Swansea University, is investigating how the properties of metal-organic frameworks, a class of materials resembling microscopic sponges, can be adjusted by taking advantage of their defects to make them better at capturing CO_2.

Dr. Taddei said: "Metal-organic frameworks, or MOFs, are extremely interesting materials because they are full of empty space that can be used to trap and contain gases. In addition, their structure can be manipulated at the atomic level to make them selective to certain gases, in our case CO_2."

"MOFs containing the element zirconium are special, in the sense that they can withstand the loss of many linkages without collapsing. We see these defects as an attractive opportunity to play with the properties of the material."

The researchers went on to investigate how defects take part in a process known as "post-synthetic exchange", a two-step procedure whereby a MOF is initially synthesized and then modified through exchange of some components of its structure. They studied the phenomenon in real time using nuclear magnetic resonance, a common characterization technique in chemistry. This allowed them to understand the role of defects during the process.

The new study appears in the high impact international journal *Angewandte Chemie*.

"We found that defects are very reactive sites within the structure of the MOF, and that their modification affects the property of the material in a unique way." said Dr. Taddei "The fact that we did this by making extensive use of a technique that is easily accessible to any chemist around the globe is in my opinion one of the highlights of this work."

ESRI Research

ESRI Director, Professor Andrew Barron is co-author of the work, said: "In ESRI, our research efforts are focused on making an impact on the way we produce energy, making it clean, safe and affordable. However, we are well aware that progress in applied research is only possible through a deep understanding of fundamentals. This work goes exactly in that direction."

The study is a proof of concept, but these findings lay the foundation for future work, funded by the Engineering and Physical Sciences Research Council. The researchers want to learn how to chemically manipulate defective structures to develop new materials with enhanced performance for CO2 capture from steelworks waste gases, in collaboration with Tata Steel and University College Cork.

"Reducing the CO2 emissions derived from energy production and industrial processes is imperative to prevent serious consequences on climate," states co-author Dr. Enrico Andreoli, Senior Lecturer at Swansea University and leader of the CO2 capture and utilization group within ESRI, "Efforts in our group target the development of both new materials to efficiently capture CO2 and convenient processes to convert this CO2 into valuable products."

Dr Taddei, Professor Barron and Dr Andreoli are the organizers of the 1st European Workshop on Metal Phosphonates Chemistry, which will be held in ESRI on the 19th of September 2018.

More information: Marco Taddei et al, Post-Synthetic Ligand Exchange in Zirconium-Based Metal-Organic Frameworks: Beware of The Defects!, *Angewandte Chemie International Edition* (2018). DOI: 10.1002/anie.201806910

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