Methane storage targets are too high

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Using natural gas for car fuel is a challenge, requiring massive research efforts to find materials that can efficiently store it. However, a Swiss-US study concludes that the best materials have not only been already discovered, but can only meet up to 70% of energy targets set by governments.

Because of its low energy density, natural gas has to be compressed or liquefied, which makes it difficult to integrate into vehicles. A popular solution is to store natural gas inside materials with nano-sized pores, and the search for such is often propelled through governmental targets. In a collaborative study, scientists have simulated over 650,000 designs for nanoporous materials, and propose that the best candidates have already been designed, meeting 70% of the US Department of Energy targets for energy storage and making additional research in this area redundant.

The study is published in *Energy & Environmental Science*.

The urgency to discover materials that can cost-effectively store methane from natural gas into cars is reflected in governmental targets such as those set by ARPA-e, an organization under the US Department of Energy. The organization wants to find a nanoporous material that can store methane with the same energy density of compressed natural gas, and do so at a lower pressure, applicable to car fuel tanks.

A computer simulation study led by EPFL and the University of California at Berkeley now suggests the best materials have already been found, and can store a maximum of 220 units of methane, which amounts to 70% of the ARPA-e target. The scientists built structure models of 650,000 different materials on the computer and rapidly prototyped them for natural gas storage using molecular simulations. These included the materials that are currently intensely explored in the field.

The scientists used the building blocks of these materials and let computers generate novel materials systematically. The performance of these materials was predicted using advanced molecular simulation techniques that were specifically developed to run on processors used in computer games with heavy graphics.

The analysis showed that it may be difficult, if not impossible, to reach the ARPA-e target for natural gas storage using nanoporous materials. Specifically, the study suggests that those targets are unrealistically high, and it predicts that the best nanoporous materials can reach an energy density up to 70% of compressed natural gas. "Of course, an interesting question that this work raises is whether one can derive such a radical conclusion based on computer simulations alone," says Berend Smit, one of the lead researchers and Director of EPFL's Energy Center.

This means that research groups around the world have already found the best nanoporous materials for methane storage. "We feel that future experimental efforts to improve this target will be a waste of time since the ARPA-e target is impossible to reach," says Smit. "Even if we find a material that is a few percent better, it will be nowhere close to the original target."

The scientists hope that their findings will prevent what might be an unnecessary research effort. As Smit explains: "We always hope that someone will discover a novel chemistry method that can reach this target, but 70% is already a major step forward and may very well be also interesting from a commercial point of view."

More information: Simon C, Kim J, Gomez-Gualdron D, Camp J, Chung YG, Martin RL, Mercado R, Deem MW, Gunter D, Haranczyk M, Sholl D, Snurr RQ Smit B. "The Materials Genome in Action: Identifying the Performance Limits for Methane Storage." *Energy Environ*. Sci. 2015, Accepted Manuscript DOI: 10.1039/C4EE03515A

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