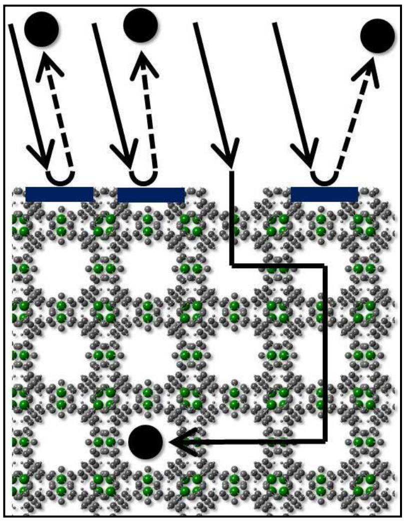
Free Pores for Molecule Transport

Researchers Identify Cause of Surface Barriers of Metal-Organic Frameworks (MOFs) – Relevant to Gas Storage



Loading of highly porous metal-organic frameworks (MOFs) that are made of metallic nodes (green) and organic connection elements (gray) with gas molecules is often inhibited by surface barriers. (Figure: IFG/KIT)

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Metal-organic frameworks (MOFs) can take up gases similar to a sponge that soaks up liquids. Hence, these highly porous materials are suited for storing hydrogen or greenhouse gases. However, loading of many MOFs is inhibited by barriers. Scientists of Karlsruhe Institute of Technology (KIT) now report in “Nature Communications” that the barriers are caused by corrosion of the MOF surface. This can be prevented by water-free synthesis and storing strategies.

MOFs are crystalline materials consisting of metallic nodes and organic connection elements. They have a very large surface area and are highly porous. Like a sponge, they can take up other molecules. MOFs, produced on a large technical scale, are highly suited for the storage of gases: When the gas enters the solid, it is partly liquefied. The density increases and much more molecules can be stored in the same volume. Among others, MOFs are suited for the storage of hydrogen in the tank of hydrogen-driven automobiles. They can also be used for storing greenhouse gases like carbon dioxide and methane. Other applications are substance separation, catalysis, and sensor technology. For any application, an appropriate MOF can be produced. Mostly, MOFs have the form of a powder. In the past ten years, more than 20,000 different representatives of this class have been synthesized and characterized in detail.

"For nearly all applications, loading of these highly porous crystals with molecules is essential," Lars Heinke of the Institute of Functional Interfaces (IFG) of KIT explains. "The efficiency of molecule transport into the porous particles is crucial to the performance of the MOFs." In many MOF materials, however, loading is inhibited largely by so-called surface barriers. The surface of the sponge is broken, the pores are clogged, and loading is delayed significantly. This limits the application opportunities.

To better understand and identify the reasons of these problems, the IFG researchers studied the formation of surface barriers. For this purpose, they conducted fundamental experiments on thin, structurally perfect MOF layers mounted on solid substrates. These SURMOFs (SURface-mounted Metal-Organic Frameworks) are characterized by a high order and ideal structure. The researchers succeeded in attributing the barriers to a corrosion of MOF layers on the surface. They demonstrated how corrosion of the surface layer proceeds and found that water plays a central role. "Many scientists thought that these surface barriers are intrinsic and, hence, cannot be prevented. This assumption has now been disproved. It is possible to produce MOFs for loading without "clogging"," says the Head of KIT's IFG, Professor Christof Wöll. The work reported in the journal "Nature Communications" refutes several previous hypotheses.

The findings might be helpful for many applications of MOFs. Due to the results of the KIT researchers, water-free synthesis strategies for MOFs will have to be developed in the future. Improved materials will ensure barrier-free transport of molecules from the gas phase and liquid phase into MOFs. This will enable to further increase the efficiency of these promising storage and functional materials.

L. Heinke, Z. Gu, and Ch. Wöll, The surface barrier phenomenon in the loading of metal-organic frameworks. Nat. Commun. 5:4462 doi: 10.1038/ncomms5562 (2014).

The Karlsruhe Institute of Technology (KIT) is a public corporation according to the legislation of the state of Baden-Württemberg. It fulfills the mission of a university and the mis-

sion of a national research center of the Helmholtz Association. Research activities focus on energy, the natural and built environment as well as on society and technology and cover the whole range extending from fundamental aspects to application. With about 9400 employees, including more than 6000 staff members in the science and education sector, and 24500 students, KIT is one of the biggest research and education institutions in Europe. Work of KIT is based on the knowledge triangle of research, teaching, and innovation.

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