R & D facts

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Office of Fossil Energy
National Energy Technology Laboratory

Chemistry and Surface Science

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Carbon Dioxide Materials Laboratory

Carbon management to prevent excessive greenhouse warming requires materials that can effectively capture carbon dioxide at point sources before sequestration. Improvements beyond current technology are needed to reduce both the cost and energy sacrifice of capture systems. New adsorbent materials show promise to overcome these barriers, but a significant amount of development work must be done to realize more efficient capture processes. In particular, one avenue to improved efficiency would be to reduce the amount of energy that must be expended to regenerate the carbon dioxide adsorbent. In this regard, solid, microporous materials offer a potential advantage over liquid adsorbents. A number of such materials are under investigation in the carbon dioxide materials laboratory including metal organic frameworks, Prussian Blue analogues, layered pillared complexes, and coordination polymers. Microporosity, high surface areas, and low heat capacities are among the favorable aspects provided by this newer generation of adsorbents. New materials are continuously being developed to solve problems in the capture and separation of carbon dioxide.

The Carbon Dioxide Materials Laboratory has the capacity to synthesize a wide variety of microporous materials suitable for capture and separation applications. Metal organic framework materials are a typical example. These materials are readily synthezied from metal ions and organic linker molecules. There is a wide range of potential structures that can be specifically designed to provide improved or novel adsorption properties. In addition to retaining carbon dioxide by simple physisorption, it is possible that introduction of specific functional groups may allow binding by stronger interaction forces. The goal is to achieve the appropriate blend of adsorption strength and ease of regeneration. In addition, by appropriate choice of building materials, the adsorbents may be readily engineered to have a wide range of pore dimensions.

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Characterization of the new materials is done by obtaining adsorption isotherms, which are critical measures of adsorption strength and capacity and are taken over a wide range of pressure and temperature. A high-resolution surface-area instrument is used that covers pressures up to one atmosphere, generally at liquid nitrogen or argon temperatures. In addition, a high-pressure instrument is used to cover pressures up to 100 atmospheres from liquid nitrogen to room temperature. Higher temperatures are available for special cases.

Direct observation of adsorbed gases is made with both infrared and Raman spectroscopy. A specially constructed variable-temperature, variable-pressure view cell obtains critical information on the specific sites responsible for adsorption. When gases are adsorbed, their infrared band is often shifted from that of free gas in a manner related to the nature of the sites it occupies. Further information on the relative binding strength of the sites is obtained from competition experiments by observing the displacement of one gas by another. The experimental results are compared with computer simulations to shed more light on the energetics of adsorption.

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