fast breaking papers - 2010

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David Sholl talks with *ScienceWatch.com* and answers a few questions about this month's Fast Breaking Paper Paper in the field of Engineering.

Article Title: Assessment of a Metal-Organic Framework Membrane for Gas Separations Using Atomically Detailed Calculations: CO2, CH4, N-2, H-2 Mixtures in MOF-5
Authors: Keskin, S;**Sholl, DS**
Journal: IND ENG CHEM RES, Volume: 48, Issue: 2, Page: 914-922, Year: JAN 21 2009
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SW: Why do you think your paper is highly cited?

Metal organic frameworks (MOFs) have generated a great deal of excitement because of the diverse range of crystalline structures than can be synthesized, but the development of large-scale applications of MOFs is only just beginning. This paper highlights a path forward for identifying MOFs that can be used as membranes to tackle some of the most important energy-related gas separations faced by today's energy industry. These are problems, like the efficient separation of methane and carbon dioxide, where new materials are needed to overcome the problems that make existing processes uneconomical.

SW: Does it describe a new discovery, methodology, or synthesis of knowledge?

The paper describes a new method for modeling MOFs for use as membranes.

SW: Would you summarize the significance of your paper in layman's terms?

New technologies that allow energy- and cost-efficient management of carbon dioxide, methane, and other gases will be critical in moving the global energy economy towards a more sustainable basis. Simply making and testing complex devices made from hundreds of variants of new materials in a laboratory is far too time-consuming to allow effective screening of new materials for these technologies.

We have developed computational modeling tools that allow us to rapidly choose the best from a large group of candidate materials for making membranes for gas separations. These tools will play an important role in focusing laboratory development and scale-up of the best materials for these important problems.

"We are working very closely with academic and industrial collaborators who are fabricating and testing membranes informed by our modeling efforts."

SW: How did you become involved in this research, and were there any problems along the way?

My group has been involved in detailed modeling of membranes for around 10 years, and we, like many others, have recently been extremely interested in understanding whether metal organic framework materials can play a productive role in this field.

SW: Where do you see your research leading in the future?

We are working very closely with academic and industrial collaborators who are fabricating and testing membranes informed by our modeling efforts. Our hope is that our work and the ongoing work of others in our community will accelerate the pace of moving towards large-scale commercial application of devices based on our ideas in generating energy and fuels.

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KEYWORDS: MOLECULAR-DYNAMICS SIMULATIONS; MIXED MATRIX MEMBRANES; MAXWELL-STEFAN FORMULATION; MONTE-CARLO SIMULATIONS; SINGLE-CRYSTAL MEMBRANE; CARBON NANOTUBES; ZEOLITE MEMBRANES; ATOMISTIC SIMULATIONS; BINARY-MIXTURES; MD SIMULATIONS.

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