

High-Performance MOFs Improve the Economics of Industrial Gases

The highly commoditized industrial gas sector relies on energy-intensive processes to produce, separate, and store industrial gases. The power required to compress gases accounts for up to 50% of the cost of the delivered gas. And, gas-separation adsorption units recover only a fraction of the feed product, necessitating processes with large waste or recycle streams.

Enter NuMat Technologies, an Illinois startup that has developed synthetic adsorbent materials to address these challenges. The company uses proprietary algorithms to design metal-organic frameworks (MOFs) for low-pressure gas storage and a unique supercritical activation technology to produce customized MOFs at industrially relevant scales.

Metal-organic frameworks, an emerging class of adsorbents, are porous crystalline structures made of metal ions (corners) linked together by organic molecules (linkers). Varying the metal corners and organic linkers allows a near-infinite number of MOFs to be made - each with different performance characteristics. This unprecedented level of tunability enables scientists to create materials with gas-separation and storage properties that are not possible with incumbent materials such as zeolites and activated carbon. In addition, MOFs can have vast internal surface areas that provide an extraordinary density of accessible adsorption sites. While the highest reported surface areas of zeolites and carbons approach 1,000 m²/g and $3,000 \text{ m}^2/\text{g}$, respectively, the current world record, which is held by MOFs that NuMat designed for gaseous hydrogen storage, exceeds $7,000 \text{ m}^2/\text{g}$ - the equivalent of 1.5 football fields

packed into each gram of material.

Industry, academia, and funding agencies have responded to the promise of MOFs with significant investments to address a range of complex storage and separation challenges. These include the integration of MOFs into low-pressure natural gas and hydrogen transportation systems, low-power carbon sequestration processes, and high-value separation units (*e.g.*, H₂/N₂, Xe/Kr). However, key commercialization challenges remain, including the complexity of designing materials, process scalability, and overall system design.

Founded at Northwestern Univ. with funding from the National Science Foundation and venture investors, NuMat has pioneered the discovery and design of MOFs. NuMat uses proprietary mathematical models to create millions of hypothetical MOF structures from starting reagents, stores these in a database, and then employs cloud computing technology to rapidly determine MOF performance — in effect, conducting centuries worth of experimentation in days. This method significantly reduces MOF development cycle time and costs, and supports a platform for producing tailor-made, applicationspecific materials. The company has also designed and produced materials for the low-pressure storage of hazardous gases. These materials have been implemented in multiple full-scale prototypes, and are undergoing testing.

For MOFs to retain their ultrahigh surface areas, innovative manufacturing processes with tight control over reaction, separation, agglomeration, and handling are needed. NuMat achieves this with its proprietary supercritical activation technology, which involves the gentle extraction of solvent from MOF pores to evacuate the material without causing structural damage. The process protects pores from being crushed, permitting the use of mechanical formation equipment, and controls particle sizes to ensure uniform mass-transfer characteristics and consistent system performance.

As a platform technology, MOFs have the potential to fundamentally transform the economics of separating, storing, and transporting gases. Industry has taken notice. Bill Kroll, chairman of Matheson TriGas and senior management director of Taiyo Nippon Sanso Corp., says his company, as a global supplier of gases and gas handling equipment, routinely monitors innovations that could advance the field. "MOFs show unique promise as an emerging material technology,

> and NuMat is at the forefront of commercializing MOF-enabled systems," he says.



▲ NuMat designs and produces MOFs porous structures comprised of metal ions (orange) linked together with organic molecules (gray, red) — for gas storage and separation. The company can produce a granulated MOF product (blue powder) using a scalable pre-pilot process with a capacity of 20 lb/day.

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