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INSIGHT

AI-BASED MATERIALS DISCOVERY:

Why Industrial Reality Must Help Shape the Future of AI-Designed Metal-organic Frameworks (MOFs)

James Stephenson
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Artificial Intelligence (AI) is increasingly heralded as the next great enabler of innovation in advanced materials. From pharmaceuticals to energy storage, AI-driven discovery offers the potential to accelerate breakthroughs that would otherwise take many years. I have often heard this described as, *"a decade of materials development in six months."*

As the chief executive officer of an early phase, industrial-scale manufacturer of metal-organic frameworks (MOFs), I share the optimism around what this new age of technology may deliver. At the same time, I see an important opportunity: ensuring that the pace of AI-driven discovery is matched by an equally strong pathway to real world deployment. Without early alignment between discovery and delivery, the journey to industrial utility may take longer than expected.

At Promethean Particles, we see collaboration with AI researchers, material scientists, and industry as essential for advancing MOF development that is both innovative and practical. Our experience in large scale, sustainable manufacturing helps bridge discovery and application, making new MOFs commercially viable. By uniting AI-driven research with industrial expertise, we believe the full potential of these materials can be realised more efficiently, more reliably, and more timely.

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THE PROMISE OF AI IN MATERIALS DISCOVERY

There is no doubt that AI-based materials discovery holds enormous promise. The ability to predict new structures, optimise properties, and simulate performance before a single experiment is run could transform traditional research and development models and economics. MOFs are materials with extraordinary potential in many climate critical, energy sensitive, applications including carbon capture, biogas upgrading, water harvesting. Therefore, the prospect of accelerating discovery is tantalising.

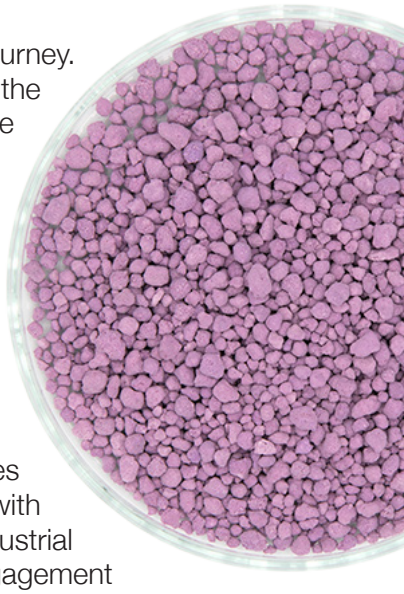
AI could help us identify structures that outperform existing benchmarks, reduce trial and error, and shorten time to market. Used effectively, it can

Promethean Particles' synthesis and characterisation lab

help focus experimental effort where it matters most, allowing researchers and manufacturers alike to move faster and with greater confidence.

EFFECTIVELY DELIVERING THAT PROMISE

The speed of adoption and expansion of AI for predicting new, higher performing MOF structures is staggering, but we are still at a very early stage of the journey. As discovery accelerates, the opportunity now is to ensure that AI progress in synthesis evolves in parallel with scalability.



AI has the potential to be a very powerful tool, but its greatest impact will come when it is combined with practical, real world insight. A lot of current MOF structures have been developed with novelty in mind rather than industrial viability. As a result, early engagement between AI-based material discovery companies and industrial manufacturers can play a valuable role in guiding effort toward structures with the strongest potential for deployment.

It is almost guaranteed that AI could help us find new combinations of exotic metals and complex organic linkers that will form new MOF structures. But the key question is how these discoveries can best support industrial adoption today. In many cases, the challenge is not discovery, but confidence in utility at industrial scale.

DO WE REALLY NEED 200,000 NEW MOFS?

Recently, a LinkedIn article celebrated the release of an open source database containing a further 200,000 new AI-generated MOF structures. While this immediately sounds like an impressive acceleration, it was less clear whether any of these new structures address specific limitations of existing materials. At this stage of the journey, value may come less from volume and more from confidence in utilisation.

In our conversations with industrial companies intrigued by the promise of MOFs, their primary needs are confidence that a material can deliver meaningful performance benefits, and

The world of MOFs has recently been set alight with the award of the Nobel Prize in Chemistry to Omar Yaghi, Richard Robson, and Susumu Kitagawa.

Since the pioneering work of these scientists first emerged more than 40 years ago, around 100,000 MOF structures have been reported.

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confidence that there are manufacturers that can produce them at a viable scale and cost without sacrificing their intrinsic quality.

The current bottleneck is therefore not a lack of structures, but commerical acceptance. Like any new solution, the use of MOFs in industrial applications will go through an improvement curve. Deployment enables learning and learning enables improvement.

INDUSTRIAL VIABILITY: WHERE DISCOVERY MEETS DELIVERY

This is where manufacturing technology can meaningfully complement AI. At Promethean Particles, we believe our capabilities can help inform AI models with practical, real world considerations. We are keen to forge strong relationships with AI companies to provide a complementary combination of structure development, synthesis feasibility, and application viability.

A scarce, expensive, toxic, rare earth metal from a conflict region does not make a great starting point for a MOF that needs to be produced at scale. Similarly, MOFs requiring complex organic linkers may face challenges unless their performance clearly justifies the cost. These are not insurmountable barriers, but they benefit from early consideration.

> *"The future of materials innovation lies where AI discovery meets industrial-scale reality, and the next step is pairing algorithms with scalable synthesis, fast feedback, and application-led testing,"*
>
> says James Stephenson, CEO of Promethean Particles.

Lastly, whilst not an impossible barrier, we ideally need MOFs that can be manufactured predominantly in water, or mild alcohol-based solvents. While traditional synthesis routes have advanced the science, there is an opportunity to explore alternatives better aligned with large scale, sustainable manufacturing.

AI models will become even more powerful when they can learn from these considerations early, not as a problem to be solved by manufacturers afterwards.

THE INTERSECTION OF AI AND PRACTICAL EXPERIMENTATION

At this early juncture, success depends on collaboration between AI innovators and industrial practitioners. Algorithms alone cannot yet tell us which MOFs will succeed in real world applications. High efficiency lab work remains essential to validate predictions and measure performance in application relevant conditions.

Dynamic CO_2 adsorption via breakthrough analysis

I long for LinkedIn posts that herald new databases of proven, industrially viable materials that solve known application shortcomings. These theory-and-practice datasets have the potential to accelerate adoption.

Promethean Particles' MATISSE carbon capture test rig

OUR ROLE IN ACCELERATING THE JOURNEY: A CALL FOR PRAGMATIC COLLABORATION

Promethean Particles is uniquely positioned to help accelerate the AI-based materials discovery process. Our continuous flow manufacturing technologies and application testing capabilities offer efficient, cost effective pathways to incorporate real world insight into discovery.

Together, we can provide the feedback loop that AI-driven discovery increasingly needs. Customers are unlikely to invest sustainably without confidence in manufacturability, scalability, and performance. By combining AI-enabled discovery with rapid synthesis and industrial insight, we can help build a more direct pathway to adoption. At Promethean Particles, we are ready to collaborate and help make that future happen.

ABOUT PROMETHEAN PARTICLES

Promethean Particles is a world-leading specialist in the synthesis and industrial production of metal-organic frameworks. Our proprietary and patented continuous flow manufacturing processes enable the industrial scale production of high-quality, cost-effective MOFs.

To discover what really determines whether a MOF can succeed at industrial scale, scan the QR code to download our white paper **Beyond CO_2 Uptake.**

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