

Designing Materials

Why AI Is Becoming a Strategic Necessity

Chemicals companies are under pressure from several directions at once: sustainability mandates that demand new formulations, supply chains that need to be reshored or diversified, and R&D budgets that are expected to deliver faster without growing larger.

Trial-and-error development, the industry's default for decades, is increasingly seen as too slow and too expensive to meet these demands alone. AI-driven materials informatics platforms have emerged as a possible solution, helping scientists mine decades of experimental data, run virtual experiments, and narrow the search space for new materials before a single sample is made in the lab. Citrine Informatics, founded in 2013, was among the first companies to build a commercial software platform around this idea, and has since worked with manufacturers across chemicals, batteries, semiconductors, and industrial materials. CHEM-

anager's Christene Smith spoke with Greg Mulholland, CEO and co-founder of Citrine Informatics, about how the market for materials informatics has matured, what still holds companies back from adopting it, and where he sees the industry heading next.

CHEManager: Citrine has been arguing that AI belongs in materials R&D since 2013, well before the current wave of AI enthusiasm. Now that every software vendor claims an AI story, how do you convince a skeptical R&D leader that this is substantively different from the hype cycle around it?

Greg Mulholland: It's been a very interesting journey, and it is exciting to see other companies pile in where we have been plugging away for a decade. We've shown the technology works and that business value can be generated. That's why there is now a market for it!

These leaders are asking the right questions, because it is sometimes hard to separate hype from reality. Fortunately, Citrine has been battle-tested over the years, and our customers are willing to talk about their success using our platform. Having them speak for us is much more convincing. You can hear from them at conferences and on our webinars and YouTube channel. You don't have to believe us.

The materials and chemicals industry has historically been slow to digitize. What has changed in the last two to three years — in the technology, the data, or the mindset of customers — that is now accelerating adoption?



Greg Mulholland, CEO & Co-Founder, Citrine Informatics

G. Mulholland: It isn't the technology or data. Our technology does continue to improve, but it really is mindset. We

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used to have to explain what machine learning is and that AI isn't science fiction. Now everyone understands that AI is the future, and they are open to it being useful.

Where do you see the greatest resistance to adopting AI-driven materials development, and is it more a technology problem, a data problem, or an organizational and cultural one?

G. Mulholland: There are a few misconceptions around AI-driven materials development that sometimes slow down adoption and implementation. The biggest is the data myth. AI first took off in industries with lots of data, for example in finance and retail where hundreds of thousands of data points are generated each day. Management magazines and courses then spoke about data as the new oil and encouraged the creation of data lakes etc. as an important first step. Materials and Chemicals are different. Our data comes from physical experiments. It's costly and time-consuming to acquire. In 50 % of projects customers start with fewer than 100 datapoints. And that's fine. We have spent a decade honing our ability to do AI on small data. Many companies waste a year or two trying to get their scientists to agree on a standard nomenclature or do data entry into a complicated system for no immediate benefit. They delay getting value from AI.

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We advocate a parallel strategy. Start with a focused AI project using the messy data you already have. Learn from it, which data is useful, and how it needs to be structured in the future. Then continue to add data to the system as you do more AI projects. That way, the scientists can see the benefit of adding data to the system, the company sees value from its data straight away, and the organization isn't taking on the cost of organizing their data only to realize that they did it in a way that isn't ideal for AI. We see this kind of wasted money and time often.

Data ownership and IP are sensitive topics when a third-party platform sits inside a company's R&D process. How has Citrine had to design its business model and technology around that trust question, and has that changed as customers have become more sophisticated?

G. Mulholland: We have always had a very simple answer to this question. We develop software. We don't develop materials. We don't own or want to own materials IP. Our business model is to sell software, and we want to be the first ones that get a call when our customers create that next market-defining material. Our customers' data is safer with us than with anyone else. We are

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ISO 27001:2022 certified. Each customer's data is private from every other's. No models are ever shared or trained between customers. We have customers who are commercial rivals. If we leaked or shared their data, it would be bad news for us and our customers. We take that responsibility very seriously.

Sustainability regulation, reshoring, and supply chain security are reshaping what materials companies need to develop and how quickly. How is that changing the kinds of problems customers bring to Citrine compared with five years ago?

G. Mulholland: The chemicals market has always had to adapt formulations because of legislation, raw material price changes, and consumer demand. I think the change over the last 5 years is urgency. Companies can't afford to wait, and AI is the only lever long enough to help move at the necessary speed. It reduces the number of experiments you need to do to hit target properties and can intelligently substitute the ingredients that everyone is trying to remove from their supply chains.

What is the biggest misconception people outside the industry have about what AI can and cannot yet do in materials science?

G. Mulholland: There seems to be an idea outside the industry that AI in materials is all about discovering brand new materials: molecules, compounds, crystals. Everyone wants the next Nobel Prize. We have worked and had success on such projects, but de novo materials discovery is only really a business in pharma. In the rest of the industry, we have to produce within current facili-

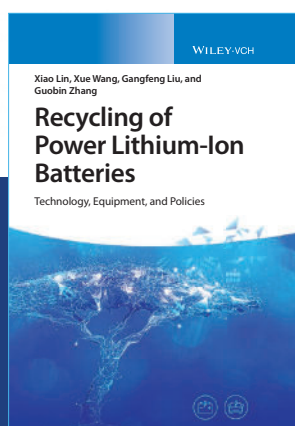
ties, at high volume, and maintain quality. Most of the projects run on our platform are for materials and chemicals that can be qualified and manufactured efficiently and sustainably this year, not for a hypothetical future where the practicalities of something totally new have all been ironed out.

If you look five to ten years out, do you expect materials informatics to become a standard, almost invisible part of how R&D is done, the way CAD became standard in engineering, or will it remain a specialized capability for companies that choose to invest in it?

G. Mulholland: It will be table stakes. Already, the top companies are not competing on whether they use AI, they are competing on how well and how broadly they use AI. It is also being used by our customers to accelerate scale-up, optimize processing, enhance yield, and improve customer responsiveness. Without AI, any margin enhancement will be off the table, and companies will be in a race to the bottom on price while the AI-enabled companies run ahead with more performant products at higher margins.

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