Advancing materials science research with AI


Credit: MaterialsZone

MaterialsZone is an R&D solution for Advanced Materials, Chemicals, and other industries that helps scientists use AI to engage with their data, merging artificial intelligence with human expertise to unlock insights from complex datasets.

In 2021, the AI cloud-based materials discovery platform MaterialsZone raised $6 million in Series A funding to develop its online materials discovery platform. MaterialsZone funnels R&D and manufacturing data into an interoperable and structured database, enabling users to achieve meaningful AI/ML insights, reduce R&D research times, and efficiently collaborate. The domain-agnostic platform can serve customers from different materials, such as energy storage, renewables, and nano-
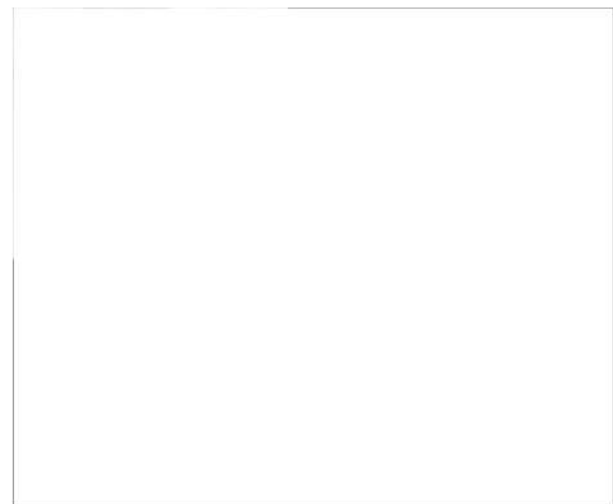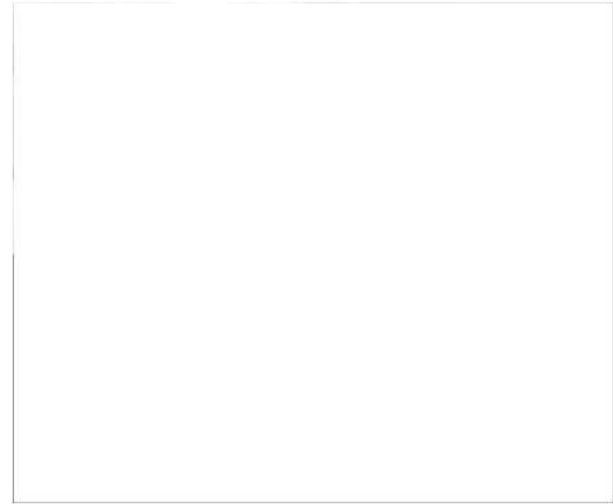
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materials, supporting simple and complex materials architectures.

Combining data within an organisation and using AI tools enables additional capabilities, such as multi-dimensional analysis, to make data-driven decisions and building models to predict experimental results.

Breakthroughs caught up with Ori Yudilevich, the CPO of MaterialsZone, to discuss how the data-driven platform is helping scientists and how GenAI tools could further bolster the capabilities of this platform in the future.

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Can you tell our readers about MaterialsZone and how the platform works?

Yudilevich: "MaterialZone is a platform that addresses the material-based products industry. We work with companies that produce products, and these products involve some kind of research in material science."

"A scientist or team of scientists develop some kind of new materials, mix different materials, or improve the processing of materials. It ranges from 3d printing to battery development, concrete, pharmaceuticals, and cosmetics. So these industries are very broad, but they have one thing in common: they design and create their products."

"They have an R&D team that does this research, and we're here to help these R&D departments, or R&D processes within companies, to accelerate their processes of discovering materials."

How does this improve existing processes?

Yudilevich: "Anybody who's been involved with AI in machine learning knows that it's about the data, and you can't get insights from your data without good quality data feeding the model. We see that as a significant challenge in materials science. These industries are often working in ways that are relatively backwards. Many of them are still documenting their R&D process in Excel spreadsheets. They're scattered all over the place, so they don't learn from iteration to iteration or from product to product."

"A researcher might do some experiments, then throw the spreadsheet somewhere, or that researcher moves on, and the next researcher comes in and doesn't know that this was done."

"MaterialsZone identified this problem many years ago, and we decided to build a data platform where scientists in these companies can aggregate all of the data related to R&D in one place, one single source of truth, or a unified database where all the data related to R&D is accessible, findable, and usable by tools that let you leverage it. And that's where AI comes in."

"This data is not only about experiments. This data is data from the whole process within a company. So it's also procurement. You want to know what materials are available. You want to know the pricing because the prices of raw materials might influence your choice. You want to know regulatory information, and you want to know even information coming from sales sometimes because some input from sales might affect the direction you'll take when developing a product."

"MaterialsZone is a data platform. It's a platform where we aggregate all the data. We call it the Materials Zone Knowledge Center. On top of this knowledge centre, we have three pillars. We have the collaboration pillar, called the Collaboration Hub, which allows people to collaborate once all the data is there. You can upload your experiments or experiment internationally because some organisations will do some tests in one place and others in

another. You can share insights with disparate teams to ensure data is not siloed."

"Then we have the Insight module. We call that the Visual Analyzer. Once you have all the data, you want to get insights from it. You want to learn. You want to look for patterns in your data and correlations between different properties."

How is AI used in this platform?

Yudilevich: "Then, we reach AI. We want to use AI and machine learning to accelerate this process. Now, the main thing is that AI doesn't replace us because there's a lot of knowledge experts in their field have accumulated throughout their careers that the AI doesn't immediately have. What AI does better than human researchers is it's capable of looking at very large parameter spaces. A human can see that A affects B, but it's hard for them to see that some combination of A, B, C and D affect E and F in some way. For machine learning, this is very natural, very simple."

"AI is designed to do that. It's not limited by brain power. MaterialsZone helps companies accelerate their development by reducing the number of experiments they want to do. Because the AI tool can look for patterns, multi-variable patterns, and help you pinpoint what experiments are worthwhile pursuing."

"The platform can save up to 60,70, or even 80% of the experiments to reach the product and go to market. That's reducing time, and it's also reducing resources because every experiment can be very costly. Typically, you do several experiments to reach a product, but that might take a few months because of expensive devices and materials."

What are the main challenges facing companies using materials science?

Yudilevich: "One problem we see repeatedly is the amount of knowledge and data out there, that is there for you to

use, is immense and very hard to get to it. One of the big problems we see people coming back with is we need help in knowing which materials or which processes we should even try to attempt."

"It's not like you have this simple recipe and just try a few things. You have a world of thousands or hundreds of thousands of possible raw materials, and after that, all the processing you can do and the use of different technologies create a complex challenge for the creation of new products.

"That information is scattered in suppliers' databases, academic literature, or patents. Having access to this data and being able to access it and link it with your workflows is a significant challenge."

"Using AI means that instead of being stuck trying out ten materials I have purchased from certain suppliers, there's also this other raw material available from a supplier, maybe far away or even nearby, that I don't know of. This material could make my product cheaper, make my product more sustainable, or make my product more fit for specific use cases. For example, if it's for food, you have different regulations limiting the type of materials you can use."

Can AI tools be innovative or help scientists to innovate in materials science?

Yudilevich: "That's a direction we're exploring right now. AI can be innovative, old-school AI and machine learning can be innovative to a certain degree. The limitation is that you programmed it. You've told it what it's playground is. What the features should look like. You can make it much more extensive than what you would try if you were a human doing the same work. Because it has a lot of CPU power and can scan much larger spaces."

"In that sense, it can be innovative, but it's not going to be innovative in the sense of discovering by chance because it's spilt something in the lab or these other amazing stories that we know from the history of science. It won't be as innovative as that, not at this stage of machine

learning. However, with the Gen AI tools, you see more of this, and that's something we're exploring."

"You can combine the existing data platform trained on your data with Gen AI. It's not that Gen AI is very creative, but it's trained on a much larger data set in such a way that we're amazed by it. This is because it seemingly knows everything. It has all this knowledge of humanity. So AI is not very innovative by itself, but humanity is innovative."

"Usually, as researchers, we don't have access to all of this knowledge, and we're working now on a tool that is a chatbot that the user can access from our platform, and it combines the power of large language models (LLMs), together with the data and the capabilities that MaterialZone has. Connecting the two enhances scientists' access to literature and available information beyond the scope of a company's internal data."

"We see these types of applications in every domain these days. How do we now specialise this general tool to a specific domain and make it very good at a specific job, such as materials science? We want AI to guide the user. To provide them with the correct recommendations. In that sense, it is innovative, and with time, we'll see more and more innovation generated by AI."
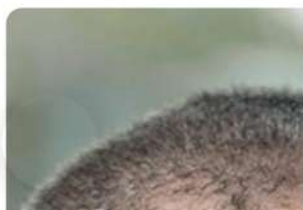
Ori Yudilevich is the CPO of MaterialsZone

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