

Tags

Climate crisis

Green energy

Technology

## Dirty, rare minerals are key for green energy to solve the climate. AI is helping us create alternative materials to kick the habit and fix the planet faster.

It has been called 'white gold' by some, and features on the energy industry's list of the world's most critical resources. Demand for the mineral has tripled since 2017 and is expected to **rise tenfold by 2050**, yet most of us don't give a second thought to the half a gram of it that we carry around in our pockets every day.

From smartphones and laptops to batteries and electric cars, lithium is key to powering not just modern connectivity but also the green energy transition.

With the planet already **breaching** the Paris Agreement's **1.5C 'tipping point' threshold**, the need to electrify the world's power supply with green energy stored and distributed via lithium materials has never been more urgent.

Lithium batteries are crucial for the green energy transition, due to their high energy density and long cycle life. It can be charged, run-down, and re-charged thousands of times without compromising its storage capacity.

But the rare earth mineral isn't free. Mining it is a dirty, carbon-intensive process in itself. Besides **international tensions** and **domestic protests**, water contamination, significant water usage, and air pollution are frequent byproducts.



*Whilst lithium plays a key role in the planet's transition to green energy, mining the rare earth mineral is a highly carbon-intensive process.*

Attempts to boost the supply of lithium have largely focused on recycling. Huge gains have been made in the industry – recyclers are now able to recover **80% of lithium** from scrap – but there's **nowhere near enough lithium scrap** to fulfil the world's ballooning lithium needs; recycling alone **isn't enough**.

Instead, scientists have been scrambling to address the shortfall through a different method: creating new alternatives.

"Chemistry is hard," explains Matthias Troyer, a technical fellow and Vice President of Quantum at Microsoft. "The challenge chemists face is having to search through trillions of potential candidates. We want to accelerate their work with a platform that every chemist can use."

Launched in June 2023, Microsoft's Azure Quantum Elements (AQE) is a scientific system that aims to do just that. Combining machine learning algorithms with enormous computing power (and, in the future, **quantum computing**), AQE aids scientists by running a range of complex calculations and simulations.

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In collaboration with scientists at the US Government's Pacific Northwest National Laboratory (PNNL), a team of researchers recently announced a breakthrough in the quest for a lithium alternative, discovering and testing a new material that can make lithium batteries up to 70% more efficient.

Creating a system for complex chemistry as intuitive a ChatGPT-style large language model is still some way off. But using today's leading AI-powered scientific tools, the research team went from screening 32 million potential materials to a shortlist of just 18 – all in a mere 80 hours. Work which previously would have taken labs decades to complete was finished off by artificial intelligence in less than a week.



*A Microsoft scientist works with the Azure Quantum Elements platform. "We want to accelerate their work with a platform that every chemist can use," says Matthias Troyer.*

"The development of novel batteries is an incredibly important global challenge," says Brian Abrahamson, Chief Digital Officer of PNNL. "Synthesising and testing materials at a human scale is fundamentally limiting. It has traditionally been a labour-intensive process."

The traditional way to discover a new, useful material requires researchers to comb through reams of scientific literature, searching for insight into how different materials may react under different circumstances; a process stymied by the incentive to publish what worked – and not what failed.

Setbacks are costly. "If it's a failure, we go back to the drawing board," says Vijay Murugesan, Material Sciences Lead at PNNL.



*Samples of the new salt-based electrolyte, N2116 discovered by Microsoft and PNNL. The material can reduce lithium use in batteries by 70%. Image: Brad DeLong.*

Artificial intelligence has completely changed the game. It's like generating a haystack and using magnets to draw out needles of insight and discovery. After lab testing, the team settled on a substance they've christened N2116. It's derived from salt, the world's most abundant resource, and is expected to reduce the lithium required in a battery by 70%. Further testing is ongoing, but a prototype has already been used to power a lightbulb.

Vijay looks forward to digitising the rest of the scientific process. "We will be able to predict how everything will work together," he predicts. "After 10,000 (recharging) cycles and five years of usage, for example, (AI) will be able to tell us what the material performance would be."

And it extends well beyond lithium, Brian adds. "Recent technology advancements have opened up the opportunity to accelerate scientific discovery. There's an opportunity to do this across every scientific field."