How the UK can lead the materials sector with AI and robotics

Professor Andrew Cooper FRS
Royal Society Research Professor, Academic Director of the Materials Innovation Factory, University of Liverpool

Artificial intelligence (AI) is a global, disruptive force. Research-active nations around the world are busily investing in AI with the hope of transforming scientific R&D. UK industry can take a lead by applying AI and robotics to key R&D areas, but this requires a differentiated national strategy.

Here, I outline research at the University of Liverpool that has led the way in physically embodied AI by using 'robot scientists' to discover new materials. This approach could revolutionise materials R&D, paving our path to net zero targets, as demonstrated with industry partners in the Materials Innovation Factory.

AI: the brain in a jar

AI is great at interpreting data but less good, so far, at coming up with entirely new concepts by itself. In some scientific research areas, we can apply AI to large, pre-existing datasets. In the physical and life sciences, the most influential example to date of AI-led research is AlphaFold, an AI system developed by Google DeepMind that accurately predicts the 3D structures of proteins from their amino acid sequences, which has applications within medicine.

This work was recognised by the 2024 Nobel Prize in Chemistry[1 2] but AlphaFold did not result from AI alone. AlphaFold was built on earlier advances in computation and structure prediction[3], and relied on a huge experimental dataset of measured and predicted protein structures, built at great cost, to train the AI mode – it did not learn protein structure for free. Also, these protein data were open and publicly available: without this, AlphaFold would have been impossible to create[4].

However, not all experimental data are open. Industry tends not to share its data in commercially competitive sectors. While greater data sharing could be facilitated by privacy enhancing technologies[5], there are some inherent limitations. For example, you cannot learn how the properties of a molecule or material correlate with its structure if you anonymise its structure because of commercial sensitivity. Additionally, even the biggest multinational companies might not possess datasets that are large enough to draw general conclusions using AI. Again, AlphaFold was based on a global effort involving 200 million openly available datasets, focussing on a narrow, albeit highly important, problem[4].

For the R&D needed to tackle other key societal challenges, the training data required to build AI models do not yet exist. Society needs new materials, for example to combat climate change, with new properties that do not exist today[6]. There are no training data available for these hypothetical materials – they must first be made in a laboratory. By itself, AI is not a panacea, especially in commercial areas, where datasets are not open, and in emerging areas of science, where few, if any, datasets exist.

Policy makers should recognise that science is not conducted 'in the cloud' – it is carried out in laboratories – and without strong and effective ways of coupling AI with our laboratories, we risk building a 'brain in a jar'.

Integrating AI with laboratory science

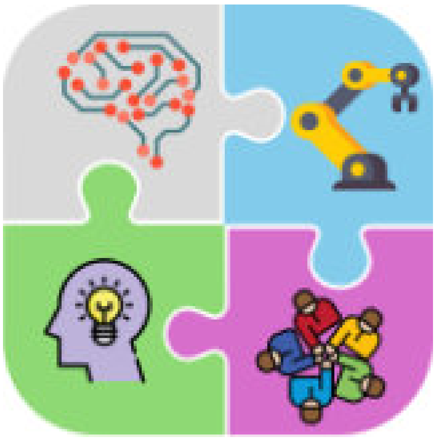
The rapid rise of open-source AI software, including software produced by large organisations such as Google and Amazon, has created a global uplift in AI capability[7]. This 'democratisation' of AI raises an important question: if everyone has it, how does the UK create a competitive advantage using AI for R&D? How do we capture the resulting value?

In the development of new scientific technologies, hard experimental data has always been the driving power. The advent of widespread AI will escalate, rather than lessen, the importance of hard data. For example, AI can make it possible to leapfrog rapidly from a new scientific discovery toward a commercially viable product, even if that initial discovery was not made using AI.

For now, at least, AI is geared more toward pattern spotting and fast optimisation, rather than genuine creativity. Therefore, these precious breakthrough discoveries become even more valuable – and potentially transient – in an era where technology development is accelerated worldwide. This creates both an opportunity and a threat for the UK.

Scientific breakthroughs can be amplified by AI and developed much faster than before, presenting a UK opportunity. Conversely, AI will make it easier for other nations to capitalise rapidly on UK-led innovation, exacerbating a challenge that predates AI. Scientific R&D is not like social media: in many areas, the commercial and societal value lies in physical products of that R&D, not the data produced along the way.

Figure 1: Competitive progress in scientific R&D cannot be solved by AI alone



The UK needs to tightly integrate cutting-edge scientific ideas (bottom left quadrant, clockwise) with AI and robotics, underpinned by teamwork and capability sharing across sectors, as in the Materials Innovation Factory at the University of Liverpool.

Figure 2: The mobile robotic chemist developed at the University of Liverpool – a physically-embodied AI agent for laboratory R&D problems

Image credit: Filip T. Szczypinski.

For these reasons, it would be a mistake for the UK to focus solely on AI capability – this could create the 'brain in a jar' scenario where the training data do not exist. However, there is huge competitive advantage in investing in the capability to produce experimental data more rapidly and integrating this tightly with emerging AI technologies (Figure 1), as we have done in the Materials Innovation Factory in Liverpool.

The most competitive long-term strategy will be to achieve this integration at the grass roots level in custom-designed facilities, rather than seeing AI as a sticking plaster that can be post-applied to existing laboratories, though there are some initial quick wins there, too. Governments, universities and industry should build this into their long-term R&D plans.

Indeed, almost all R&D-intensive industries already have their own 'lab of the future' programmes, although some are mostly conceptual so far. Having spoken to the leads of many such programmes, I see huge commonalities between different industry sectors, both in terms of the drivers and the perceived barriers to implementation. For one thing, the breakneck pace of AI and robotics development means that all 'lab of the future' programmes are shooting at a rapidly moving target.

Unleash the data-bots!

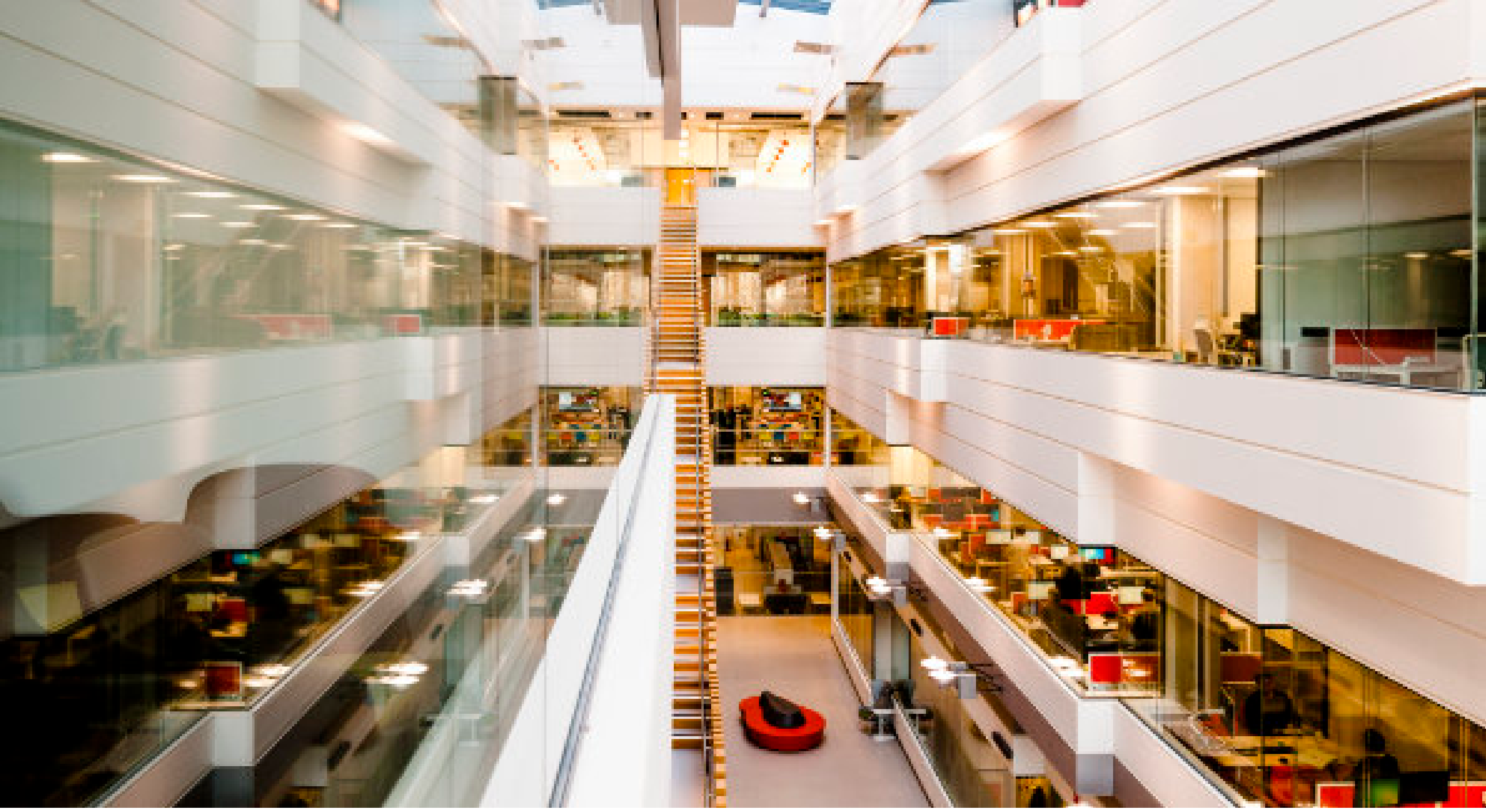
In the Materials Innovation Factory at the University of Liverpool, we addressed the challenge of fast experimental data creation by building the world's first 'mobile robotic chemist'[8 9]. Inspired by global net zero targets, this robot was built to search for clean energy catalysts, carrying out autonomous experiments over the course of days or weeks (see videos in reference 8).

The robot performed experiments at a rate that was at least 200 times faster than a human researcher[8] – effectively, doing a PhD in a week – while using an AI algorithm to decide which experiments to do next, without any human intervention. In an eight-day, 24/7 continuous search, the autonomous robot discovered a catalyst that was six times better than the composition that we started with. This is the tightest possible coupling of AI with experimental R&D, and the embodiment of the scheme in Figure 1: that is, the AI updates its beliefs around the clock, folding in new experimental data as soon as they are obtained, before telling the robot what to do next, based on initial ideas and targets set by a human research team.

From a scalability perspective, this approach leverages the rapidly declining cost of industrial robotics[10]. Moreover, essentially all scientific R&D equipment is designed to be used by human researchers, and this represents an enormous installed capital base worldwide. Likewise, all laboratories are built to a human scale. The use of an anthropomorphic, roughly human-sized robot scientist (Figure 2) means that we have a drop-in solution that can be used in existing facilities, sharing key equipment with human researchers if needed[11].

This robotic approach is applicable to multiple R&D sectors, just as industrial robots have already found applications in multiple manufacturing sectors. For example, we already have examples in pharmaceutical research[11] and consumer products. As well as greatly accelerating existing R&D, this technology will also allow companies to tackle high-risk, high-reward goals where current methodologies are just too slow to justify the time and resource commitment.

Researchers at the University of Liverpool are also working to make these robots smarter with more advanced AI. For example, we are researching agent-based methods where AI can make more nuanced interpretations of laboratory measurements[11], reason about chemical composition[12], and fold human scientific hypotheses into the optimization loop[13], with the long-term aim of building a



The Materials Innovation Factory at the University of Liverpool – a unique space that is shared by industry and university researchers with a common interest in using AI and robotics to find better materials

hybrid intelligence that combines the best aspects of AI and human reasoning.

Our aim is not to replace human teams with AI – indeed, the premium on human scientific creativity has never been higher than today. Rather, we see AI as a tool that will allow the UK to develop new scientific discoveries on a timescale that is competitive with global challenges such as climate change and net zero.

The Materials Innovation Factory

Our vision of directly coupling AI to robotic R&D laboratories (Figure 1) is applicable both to university and industrial research programmes. A live example of this is the Materials Innovation Factory (MIF) that we established at the University of Liverpool in 2017. The MIF is a globally unique facility that is shared by both academic and industry researchers. Our key partner Unilever filed 200 patents between 2020 and 2022 based on data generated at MIF, and they invested more than €100 million in this innovation hub in the three-year period 2020–2023[14]. What's more, the MIF was highlighted in a recent paper by the Tony Blair Institute for Global Change as a national strength for the UK[15]. The MIF is also one of the co-leads in the EPSRC-funded £12 million AI for Chemistry Hub, Alchemy, which aims to catalyse the use of AI in chemistry in the UK[16].

References

[1] Nobel Prize in Chemistry 2024. www.nobelprize.org/prizes/chemistry/2024/summary

[2] J Jumper et al. (2021) Highly accurate protein structure prediction with AlphaFold. *Nature* 596: 583–589.

[3] B Kuhlman, et al. (2003) Design of a novel globular protein fold with atomic-level accuracy. *Science* 302: 1364–1368.

[4] EMBL (2023) *Case study: AlphaFold uses open data and AI to discover the 3D protein universe*. www.embl.org/news/science/alphafold-using-open-data-and-ai-to-discover-the-3d-protein-universe

[5] The Royal Society (2024) *Science in the Age of AI: How artificial intelligence is changing the nature and method of scientific research*. https://royalsociety.org/-/media/policy/projects/science-in-the-age-of-ai/science-in-the-age-of-ai-report.pdf

[6] Q Gibson et al. (2021) Low thermal conductivity in a modular inorganic material with bonding anisotropy and mismatch. *Science* 373: 1017 www.science.org/doi/10.1126/science.abh1619

[7] Sahota N (2024) *AI Democratization: Turning the Tables on Tech Exclusivity*. www.neilsahota.com/ai-democratization-turning-the-tables-on-tech-exclusivity

[8] B Burger et al. (2020) A mobile robotic chemist. *Nature* 583: 237–241. www.nature.com/articles/s41586-020-2442-2

[9] BBC News feature (2020). www.youtube.com/watch?v=WBwZp5Bg2L8

[10] Inbolt (2024) *Industrial Robot Cost Decline*. www.inbolt.com/resources/industrial-robot-cost-decline

[11] T Dai et al. (2024) Autonomous mobile robots for exploratory synthetic chemistry *Nature* 635: 890–897. www.nature.com/articles/s41586-024-08173-7

[12] J Clymo et al. (2025) Exploration of Chemical Space Through Automated Reasoning. *Angewante Chemie International Edition* 64, e202417657. https://onlinelibrary.wiley.com/doi/epdf/10.1002/anie.202417657

[13] Cissé A et al. (2025) HypBO: accelerating black-box scientific experiments using experts hypotheses. *Proceedings of the 33rd International Joint Conference on Artificial Intelligence. (IJCAI-24)*, 3881 www.ijcai.org/proceedings/2024/0429.pdf

[14] Unilever (2023) *How Robots Help Design our Beauty Products*. www.unilever.com/news/news-search/2023/how-robots-help-design-our-beauty-products

[15] Boakye B et al. (2025) *A New National Purpose: Accelerating UK Science in the Age of AI*. London: Tony Blair Institute for Global Change. https://institute.global/insights/tech-and-digitalisation/a-new-national-purpose-accelerating-uk-science-in-the-age-of-ai

[16] Alchemy website. https://aichemy.ac.uk