# Artificial Intelligence, Scientific Discovery, and Product Innovation*

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This paper studies the impact of artificial intelligence on innovation, exploiting the randomized introduction of a new materials discovery technology to 1,018 scientists in the R&D lab of a large U.S. firm. I find that AI-assisted researchers discover 44% more materials, resulting in a 39% increase in patent filings and a 17% rise in downstream product innovation. These compounds possess more novel chemical structures and lead to more radical inventions. However, the technology has strikingly disparate effects across the productivity distribution. The bottom third of scientists see little benefit, while the output of top researchers nearly doubles. To understand the mechanisms behind these results, I investigate the dynamics of the human-AI collaboration. AI automates 57% of "idea generation" tasks, reallocating researchers to the new task of evaluating model-produced candidate materials. Differences in discernment ability explain the tool's heterogeneous impact: top scientists leverage their domain knowledge to prioritize promising AI suggestions, while others waste significant resources testing false positives. Together, these findings demonstrate the potential of AI-augmented research and highlight the complementarity between algorithms and expertise in the innovative process. Survey evidence reveals that these gains come at a cost, however, as 82% of scientists report reduced satisfaction with their work due to decreased creativity and skill underutilization.

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# 1 Introduction

The economic impact of artificial intelligence will depend critically on whether AI technologies not only transform the production of goods and services, but also augment the process of innovation itself (Aghion et al., 2019; Cockburn et al., 2019). Recent advances in deep learning show promise in generating scientific breakthroughs, particularly in areas such as drug discovery and materials science where models can be trained on large datasets of existing examples (Merchant et al., 2023; Mullowney et al., 2023; DeepMind, 2024). Yet little is known about how these tools affect invention in a real-world setting, where R&D bottlenecks, organizational frictions, or lack of reliability may limit their effectiveness. As a result, the implications of AI for both the pace and direction of innovation remain uncertain. Moreover, the consequences for scientists are ambiguous, hinging on whether AI technologies complement or substitute for human expertise.

To provide evidence on these questions, I exploit the randomized introduction of an AI tool for materials discovery to 1,018 scientists in the R&D lab of a large U.S. firm. The lab focuses on applications of materials science in healthcare, optics, and industrial manufacturing, employing researchers with advanced degrees in chemistry, physics, and engineering. Traditionally, scientists discover materials through an expensive and time-consuming system of trial and error, conceptualizing many potential structures and testing their properties. The AI technology leverages developments in deep learning to partially automate this process. Trained on the composition and characteristics of existing materials, the model generates "recipes" for novel compounds predicted to possess specified properties. Scientists then evaluate these candidates and synthesize the most promising options. Once researchers create a useful material, they integrate it into new product prototypes that are then developed, scaled, and commercialized.

The lab rolled out the model in three waves starting in May of 2022. Teams of researchers were randomly assigned to waves, allowing me to identify the effects of the technology by comparing treated and non-yet-treated scientists. Using detailed data on each stage of R&D, I study the impact of AI on materials discovery and the downstream effects on patenting and product innovation.

AI-assisted scientists invent 44% more materials. These compounds possess superior properties, revealing that the model also improves quality. This influx of materials leads to a 39% increase in patent filings and, several months later, a 17% rise in product prototypes incorporating the new compounds. Accounting for input costs, the tool boosts R&D efficiency by 13-15%. These results have two implications. First, they highlight the potential of AI-augmented research. Second, they confirm that these discoveries translate into product innovations, not fully bottlenecked by later stages of R&D.

AI accelerates the pace of innovation, but how novel are these breakthroughs? A key concern with using machine learning for science is its potential to amplify the "streetlight effect" (Khurana, 2023; Kim, 2023; Hoelzemann et al., 2024). Because models are trained on existing knowledge, they might direct search toward well-understood but low-value areas. Contrary to this hypothesis, I find that AI increases novelty in all three stages of R&D. I first measure the originality of new materials themselves, following the chemical similarity approach of De et al. (2016). Compared to existing compounds, model-generated materials have more distinct physical structures, suggesting that AI unlocks new parts of the design space.[1] Second, I show that this leads to more creative inventions. Patents filed by treated scientists are more likely to introduce novel technical terms—a leading indicator of transformative technologies (Kalyani, 2024). Third, I find that AI changes the nature of products: the tool boosts the share of materials integrated into new product lines rather than improvements to existing ones, engendering a shift toward more radical innovation (Acemoglu et al., 2022a).

Next, I show that the tool disproportionately benefits high ability scientists. I construct a measure of initial productivity based on discoveries in the pre-treatment period. To account for the possibility that certain compounds are inherently easier to discover, I control for material type and application.[2] Estimating separate treatment effects for each productivity quantile, I document strikingly disparate impacts across the ability distribution. The bottom third of researchers see minimal gains, while the output of top scientists increases by 81%. Consequently, 90:10 performance inequality more than doubles. This suggests that AI and scientific expertise are complements in the innovation production function.

The second part of the paper investigates the mechanisms behind these results, exploring the dynamics of the human-AI collaboration. Combining rich text data on scientist activities with a large language model to categorize them into research tasks, I show that AI dramatically restructures the innovative process. The tool automates 57% of "idea generation" tasks, reallocating scientists to the new task of evaluating AI-suggested compounds. In the absence of AI, scientists devote nearly half their time to conceptualizing potential materials. This falls to less than 16% after the tool's introduction. Meanwhile, effort on evaluation tasks rises three fold. AI therefore has countervailing effects: while it replaces labor in the specific activity of designing candidate materials, it augments labor in the broader discovery process by creating new tasks. Moreover, consistent with task-based theories of technical change (Acemoglu and Autor, 2011; Acemoglu

[1] I support this finding with survey evidence. Scientists report that materials suggested by the model tend to be more distinct than those discovered using traditional methods.

[2] The resulting metric is correlated with intuitive scientist characteristics such as tenure in the lab and attending a top university, suggesting that it indeed captures a notion of research ability.

and Restrepo, 2018), this reallocation effect is stronger for scientists with an initial comparative advantage in evaluation.

Next, I show that scientists' differential skill in assessing AI-generated compounds explains the tool's heterogeneous impact. I collect data on the compounds researchers test and the outcomes of these experiments. Top scientists leverage their expertise to identify promising AI suggestions, enabling them to investigate the most promising candidates first. In contrast, others waste significant resources testing false positives. Indeed, a significant minority of researchers prioritize AI-generated designs no better than random chance, seeing little benefit from the tool. Discernment ability is positively correlated with initial productivity, explaining the widening inequality between scientists. These results demonstrate the growing importance of a new research skill—evaluating model predictions—that complements AI technologies.

To understand these large differences in judgement, I conduct a survey of the lab's researchers. The responses reveal the central role of domain knowledge: scientists skilled in discernment credit their training and experience with similar materials as key to their assessment process, while those who struggle to evaluate AI-suggested compounds find that their background offers little assistance. While some have posited that big data and machine learning will render domain knowledge obsolete (Anderson, 2008; Gennatas et al., 2020), these results show that only scientists with sufficient expertise can harness the power of AI.

I combine my estimates with a task model to illustrate how organizational adaptation can amplify the tool's impact. AI changes the returns to specific skills, increasing the value of discernment while reducing the importance of idea generation. Therefore, adjusting hiring and firing practices to prioritize researchers with strong discernment skills implies significant productivity gains. In the final month of my sample—excluded from the primary analysis—the firm restructured its research teams. Consistent with the theory, this resulted in a higher proportion of skilled evaluators.

The consequences of new technologies extend beyond productivity. They can profoundly affect worker wellbeing and the expertise needed to succeed on the job (Nazareno and Schiff, 2021; Soffia et al., 2024). These considerations are particularly salient in the context of innovation, as they mediate AI's impact on who becomes a scientist, the fields they enter, and skills they invest in. The final part of the paper explores these questions using the survey.

Researchers experience a 54% reduction in satisfaction with their tasks. This effect is fairly uniform across scientists, showing that even the "winners" from AI face costs. Respondents cite skill underutilization and reduced creativity as their top concerns, highlighting the difficulty of adapting to rapid technological progress. Moreover, these results challenge the view that AI will primarily automate tedious tasks, allowing humans to focus on more rewarding activities. While

enjoyment from improved productivity partially offsets this negative effect, especially for high ability scientists, 82% of researchers see an overall decline in wellbeing.

In addition to impacting job satisfaction, working with the tool changes materials scientists' views on artificial intelligence. Belief in the ability of AI to enhance productivity nearly doubles. At the same time, concerns over job loss remain constant, reflecting the new tasks created by the model. As a result of the changing research process, scientists increasingly believe that AI will change the skills needed to succeed in their field. Consequently, the number of researchers planning to reskill rises by 71%. These findings show that hands-on experience with AI can profoundly influence views on the technology. The responses also reveal an important fact: domain experts did not anticipate the effects documented in this paper.

While my study focuses on materials science, the insights may apply more generally to fields where the discovery process requires search over a vast but well-defined technological space. This characterizes areas where the foundational principles are known, but complexity makes it challenging to identify specific instances. In drug discovery, for example, the properties of atomic bonds are well established, but the large number of possible chemical configurations makes the problem extremely difficult. Deep learning models—which excel in extracting features from complex data—have the potential to transform research in such settings (Hassabis, 2022). Beyond materials science and pharmaceuticals, several economically important fields fall into this category, including structural biology (Jumper et al., 2021; Abramson et al., 2024; Subramaniam, 2024), genomics (Caudai et al., 2021), climatology (Kochkov et al., 2024), and even certain parts of mathematics (Tao, 2024; Trinh et al., 2024).

**Related Literature** This paper contributes to four related literatures. First, it adds to a large body of evidence on the consequences of new technologies for productivity, labor demand, and organizations (Autor et al., 1998; Athey and Stern, 2002; Bresnahan et al., 2002; Autor et al., 2003; Bloom et al., 2014; Autor, 2015; Garicano and Rossi-Hansberg, 2015; Webb, 2020; Acemoglu and Restrepo, 2022; Agrawal et al., 2019; Acemoglu et al., 2022b; Kogan et al., 2023; Autor et al., 2024). While these studies focus on the production of goods and services, I consider a breakthrough that augments the process of innovation itself. In standard models, technologies that automate production tasks have qualitatively different effects than those performing research tasks, given the compounding social returns to innovation (Aghion et al., 2019; Jones and Summers, 2020). Therefore, understanding the implications of AI for R&D is of central importance.[3] Indeed, my

[3]A recent debate centers around the potential macroeconomic impacts of AI (Bostrom, 2014; Brynjolfsson and Unger, 2023; Clancy and Besiroglu, 2023; Erdil and Besiroglu, 2023; Ramani and Wang, 2023; Schulman, 2023; Aschenbrenner, 2024; Chow et al., 2024; Korinek and Suh, 2024). While these papers agree that a central factor is the extent to which AI

results suggest that analyses of AI that do not consider effects on science and innovation (e.g., Acemoglu, 2024) may be incomplete.[4]

Second, I contribute to recent evidence on the productivity effects of "generative" AI. This literature studies the application of large language models to mid-skill writing and coding tasks, finding that LLMs boost average output and compress the productivity distribution (Brynjolfsson et al., 2023; Dell'Aqua et al., 2023; Noy and Zhang, 2023; Peng et al., 2023). I analyze the adoption of a different type of generative model—one that produces novel material designs rather than words. While I similarly observe large gains in performance, AI is most useful to high-ability scientists in my setting, increasing inequality. This suggests that the so-called "leveling-up" effect is context-dependent and not a general feature of AI technologies. Moreover, since the model unlocks breakthroughs beyond the capabilities of even highly trained scientists, my findings help alleviate concerns that AI will contribute only to low-value tasks (Angwin, 2024).

Third, I relate to work on human-AI collaboration, particularly the relationship between algorithms and expertise (Kleinberg et al., 2017; Chouldechova et al., 2018; Cowgill, 2018; Cheng and Chouldechova, 2022; Donahue et al., 2022; Leitão et al., 2022; Mullainathan and Obermeyer, 2022; Alur et al., 2023; Angelova et al., 2023; Agarwal et al., 2024; Alur et al., 2024; Gruber et al., 2024). Scientists in my setting display considerable variation in their ability to evaluate AI-suggested compounds. Discretion boosts discovery rates for two-thirds of scientists, who leverage their domain knowledge to improve upon the model. This shows that these experts observe certain features of the materials design problem not captured by the algorithm. In contrast, a significant minority of scientists experience little benefit from the technology due to poor discerment. This dichotomy highlights the need for further research on human-AI collaboration in generative tasks.

Finally, I add to a nascent literature on the implications of artificial intelligence for science and innovation (Cockburn et al., 2019; Agrawal et al., 2023; Besiroglu et al., 2023; Ludwig and Mullainathan, 2024; Manning et al., 2024; Mullainathan and Rambachan, 2024). This paper provides the first causal evidence of AI's impact on real-world R&D. I show that AI can automate the critical ideation step of the materials discovery process, leading to an increase in invention and a rise in product innovation. Moreover, I quantify the effect of this automation on scientists, revealing a dramatic reallocation across research tasks. Consequently, I establish a micro-foundation for the recent finding that investments in AI technologies predict subsequent firm growth (Babina et al., 2024).

will accelerate innovation, lack of empirical evidence on this key variable has prevented concensus.

[4] Acemoglu (2024) expects that significant impacts of AI on overall science and innovation are more than a decade away. While my results do not directly speak to such aggregate effects, they do show that AI technologies can already contribute to R&D in specific settings.

**Organization** The paper is structured as follows. Section 2 provides information on the setting, detailing the materials science R&D process and the AI technology. Section 3 describes the data, measurement strategy, and research design. Section 4 presents the main results on discovery, patenting, and product innovation. Section 5 analyzes heterogeneity in the effect of AI across scientists and Section 6 studies the dynamics of the human-AI collaboration. Section 7 explores the tool's impact on scientists' job satisfaction and beliefs about AI. Section 8 concludes.

# 2 Setting and Background

## 2.1 Materials Science R&D Lab

My setting is the R&D lab of a large U.S. firm. The lab specializes in materials science, a field that integrates insights from physics, chemistry, and engineering to create novel substances and incorporate them into products. Often deemed the "unsung hero" of technological progress, advances in materials science underpin many significant breakthroughs (Diamandis, 2020). The purification of silicon in the 1950s enabled the development of integrated circuits, laying the foundation for modern computing. Graphene, a crystalline carbon lattice created in 2004, has transformed numerous products ranging from batteries to desalination filters. More recently, novel photovoltaic structures have enhanced solar panel efficiency, driving the steep decline in renewable energy costs. And in medicine, biocompatible compounds allow implants to merge seamlessly with human tissue, improving drug delivery systems. Moskowitz (2022) estimates that more than two thirds of new technologies rely on innovative materials, highlighting the field's economic importance.

The lab in my study focuses on applications of materials science in healthcare, optics, and industrial manufacturing, producing a wide range of patents and product innovations. To create these technologies, the firm employs thousands of highly trained scientists with advanced degrees in chemical engineering, physics, and materials science. Researchers are organized in teams, specializing in material-application pairs relevant to their expertise. These groups also include support staff such as technicians and administrators.

Figure 1 summarizes the R&D pipeline. First, scientists define a set of target properties and generate ideas for new compounds predicted to satisfy these requirements. Before the introduction of AI, researchers employed a combination of domain knowledge and iterative computational procedures to create preliminary designs. Given the difficulty of predicting material characteristics, this process is time-intensive and involves many false positives (Reiser et al., 2022).

Next, scientists evaluate candidate compounds and decide which to test. Experiments are costly,

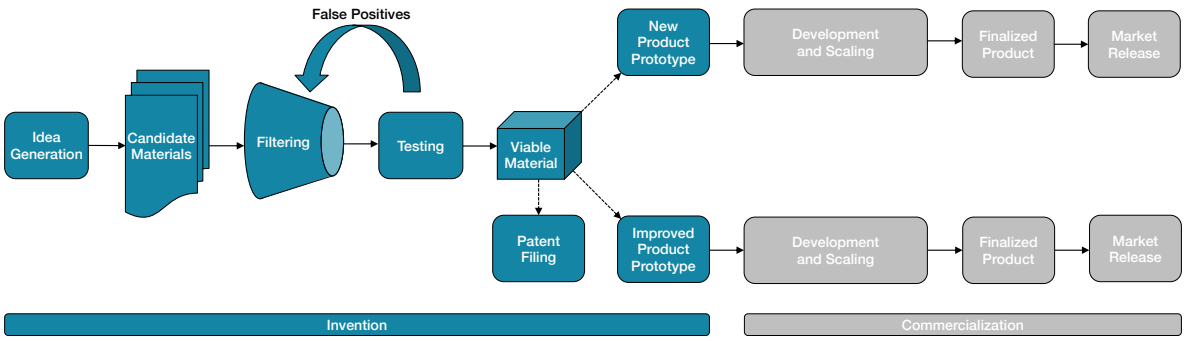



**Figure 1.** Materials Science R&D Pipeline

*Notes:* This figure summarizes the materials science R&D pipeline. First, scientists generate new compound designs. Next, they filter these candidate materials and test the most promising. After a viable material is discovered, scientists typically file for a patent and incorporate it into new product prototypes. Finally, these prototypes are developed, mass-produced, and released to market. My analysis focuses on the "invention" steps, depicted in blue.

so prioritization is key to efficiency.[5] Researchers identify promising compounds using simulations and prior experience with similar materials. Once the lab selects a candidate for testing, they advance it through a series of experiments. First, they attempt to synthesize the material, ruling out a large share of candidates that do not yield stable compounds. Next, they conduct tests to assess its properties at both the atomic and macro scales. Finally, they subject it to real-world conditions such as heat, pressure, or human interaction.

After discovering a material, scientists often file for a patent. This can pertain to a single compound, a combination of compounds, or a new technology that utilizes them. Patents require three criteria: novelty, utility, and non-obviousness. As a result, they mark the stage of research where a scientific discovery transforms into a useful invention. Patent applications typically take two years for approval, so my analysis focuses on filings. Historically, more than 80% of the lab's applications have been approved.

Finally, the lab integrates new materials into products. These could represent entirely new product lines or improvements to existing ones. In either case, researchers first develop a prototype that is then advanced through development and mass production. The "commercialization lag" between the creation of a working prototype and its market release can be substantial, ranging from years to decades.[6] Consequently, my analysis focuses on the prototyping stage. This paper's results should therefore be understood as reflecting the "invention" component of R&D (Budish et al., 2015).

[5]For example, the machines used to grow crystal structures are extremely capital-intensive and require costly inputs for each use.

[6]The length of this delay depends on several factors, including the regulatory environment and the process for manufacturing materials at scale.

## 2.2 Deep Learning for Materials Discovery

Materials discovery is challenging due to its complexity. The space of plausible chemical configurations is vast, requring scientists to explore a large number of potential compounds. Moreover, while the properties of atomic bonds are well known, it is difficult to predict how they will aggregate into large-scale characteristics. Deep learning models—which excel in extracting features from complex data—have the potential to overcome these challenges (Hassabis, 2022).

Recent years have seen an explosion of large, standardized databases compiling the structure and characteristics of known compounds. Combined with algorithmic progress and increased compute, this has greatly improved the performance of deep learning in materials science (Reiser et al., 2022). As a result, the field has shown rapidly growing interest in these techniques.

Figure 2 illustrates the rise of deep learning in materials science. Over the past four years, the number of materials science publications referencing deep learning has grown by 437%. This follows a decade of foundational progress in the computer science literature.[7] At the same time, deep learning has become integrated into materials science curricula, evidenced by a sharp increase in PhD syllabi covering these methods.

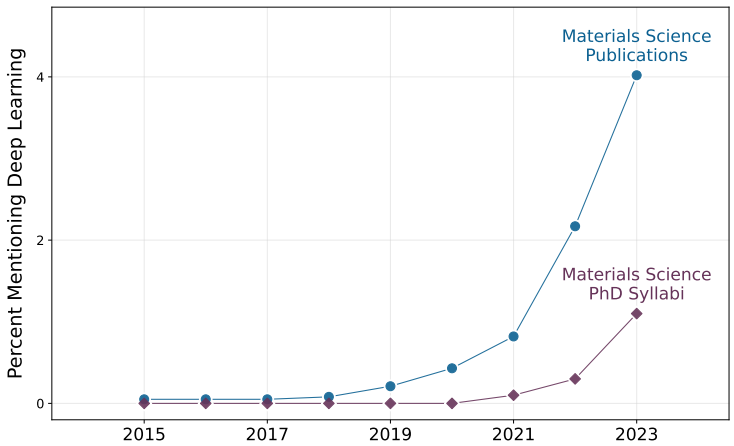



**Figure 2.** The Rise of Deep Learning in Materials Science

*Notes:* This figure documents the rise of deep learning in materials science. The blue circles show the percent of materials science publications mentioning deep learning. This information comes from Web of Science (`https://www.webofscience.com/wos/woscc/basic-search`). The purple diaomonds plot the percent of materials science PhD syllabi covering deep learning. These data come from Open Syllabus (`https://www.opensyllabus.org/`).

[7] Seminal papers include Goodfellow et al. (2014); Mirza and Osindero (2014); Radford et al. (2016); Arjovsky et al. (2017); Karras et al. (2018).

## 2.3 AI Tool

The lab's AI technology is a set of graph neural networks (GNNs) trained on the structure and properties of existing materials. Introduced by Scarselli et al. (2009), GNNs extend generative models to settings where geometric structure contains essential information.[8] The GNN architecture represents materials as multidimensional graphs of atoms and bonds, enabling it to learn physical laws and encode large-scale properties.

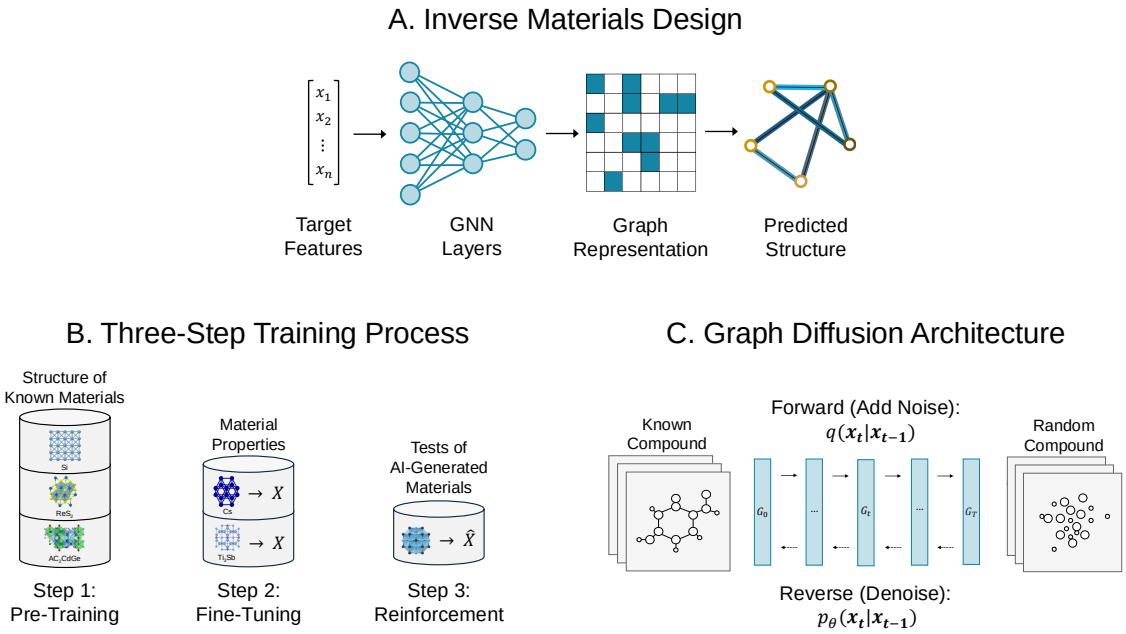



**Figure 3.** Illustration of Materials Discovery Tool

*Notes:* This figure describes the structure of the lab's AI tool. The graph neural network is input a set of target features and outputs a predicted structure (Panel A). The model is trained in three steps: pre-training based on the structure of known materials, fine-tuning for a specific application based on material properties, and reinforcement learning based on scientists' experiments on AI-generated compounds (Panel B). It generates stable materials by reversing a corruption process, iteratively denoising an initially random structure (Panel C).

Scientists use the tool for "inverse materials design," illustrated in Figure 3, Panel A. Researchers input a set of desired characteristics and the model generates candidate compounds predicted to possess these properties (Zunger, 2018; Noh et al., 2020). The model undergoes three stages of training to optimize its performance: pre-training on a large dataset of known structures, fine-tuning with application-specific material properties, and reinforcement learning using tests of model-suggested compounds (Panel B). It employs a diffusion-based approach to generate novel materials. The model begins with a known structure, adds noise, and then reverses the

[8] Foundational papers on graph neural networks include Henaff et al. (2015), Johnson (2017), Kipf and Welling (2017), Li et al. (2018), and Velickovic et al. (2018).

process to create a new compound (Panel C). While AI designs have the potential to rapidly advance discovery, materials proposed by even frontier models are often unstable or display other undesirable features.[9] Consequently, it is essential to pair the technology with scientists who can evaluate, refine, and test candidate compounds.

### 2.4 Model Rollout

Following a short pilot program, the lab began a large-scale rollout of the model in May of 2022. They randomly assigned teams of researchers to three adoption waves spaced approximately six months apart. The firm randomized deployment due to uncertainty about the tool's impacts and to determine if they should alter hiring and training practices.[10] The treatment groups were comprised of 404, 419, and 195 scientists, respectively. At the start of each wave, researchers participated in a training program teaching them how to use the technology. My analysis focuses on the three main treatment groups, totaling 1,018 scientists across 221 teams.

## 3 Data, Measurement, and Research Design

### 3.1 Data and Measurement

I combine several data sources to create a uniquely detailed picture of the R&D process. Appendix B provides a full description of variable definitions, sample construction, and measurement procedures.

**Materials** I collect data on candidate compounds, synthesized substances, and finalized materials. These include information on compounds' physical structure, captured by the composition and geometric orientation of their atoms and bonds. Additionally, I observe the results from tests of material properties, providing a large set of characteristics at the atomic and macro scales.

I classify new materials as "discovered" once they are added to the lab's internal database of compounds deemed viable for product use. This marks the transition from science to engineering, after which the materials are developed and produced at scale. I link compounds to the scientists that create them. Because researchers collaborate in teams, many materials are credited to multiple scientists. However, not all team members work on every material their team discovers.

[9] For example, an anaysis of 2.2 million crystal structures discovered by DeepMind's AI tool found "scant evidence for compounds that fulfill the trifecta of novelty, credibility and utility" (Cheetham and Seshadri, 2024).

[10] To my knowledge, no changes to hiring and training were made during the course of the experiment. Nevertheless, I exclude new hires from my main analysis.

I measure the quality of compounds based on their properties. Scientists begin the search process by defining a set of target features. These features vary signifiantly across materials, but often include both atomic and large-scale characteristics determined by the intended application. For example, researchers may target the band gap (the energy difference between the valence and conduction bands) or the refractive index (how much a material bends light). For each feature, I calculate the distance between the target and its realized value. Following the materials science literature, I combine these distances into three indices: one capturing quality at the atomic scale, another at the macro scale, and a third that combines all properties into a single index. Appendix B.2 details the construction of these indices.

To assess the novelty of materials, I employ the chemical similarity approach of De et al. (2016). This method is similar in spirit to the procedure used by Krieger et al. (2021) to measure the novelty of pharmaceutical drugs. However, it includes additional features necessary for studying the inorganic compounds in my setting. Premised on the idea that "form determines function," it defines the innovativeness of a new material by comparing its physical structure to existing compounds. The similarity measure captures both the set of elements in a compound and their geometric orientation. I compare each discovered compound to the more than 150,000 materials in the Materials Project and Alexandria databases (Jain et al., 2013; Schmidt et al., 2022). This methodology applies only to crystal structures, solids with orderly and periodic atomic arrangements. The novelty results are therefore based solely on the crystals in my sample, comprising 64% of all materials. Appendix B.3 describes the similarity measure in detail.

**Patent Filings** I match new materials to patent filings. I include patents for both compounds themselves and technologies that utilize them. Given that patent applications take approximately two years for approval, my results focus on filings rather than approvals. Historically, more than 80% of the lab's applications have been approved. The patent data are useful for two reasons. First, patents identify inventions as significant, applicable breakthroughs. Second, the text of patent filings allows me to assess the novelty of inventions using similarity measures.

The first similarity measure, proposed by Kelly et al. (2021), captures a broad notion of novelty using the full text of patent filings. It quantifies textual similarity using the cosine similarity between vectors of term frequencies. To appropriately weight terms by their importance, each component is scaled by the inverse frequency of that term in the full sample. The resulting metric lies in the interval $[0, 1]$, where patents using the exact same words in the same proportion have similarity of one and patents with no common terms have similarity of zero.

Following Kalyani (2024), the second measure of patent novelty focuses solely on the introduction of new technical terms. It converts the text of patent filings into bigrams—word pairs such

as "phase transition" or "thermal conductivity." After removing non-technical terms, it defines the novelty of a patent as the share of bigrams that do not appear in any previous patent. As show by Kalyani (2024), this is a leading indicator of transformative technologies. In my sample, patents contain an average of 544 technical bigrams. Out of these, 6.28% are classified as new terms. Appendix B.4 details the construction of the patent similarity measures.

**Products** To assess downstream innovation, I gather data on products incorporating newly discovered materials. I observe how the material is used and whether the product represents a new line or an improvement to an existing one. I measure product innovations based on the creation of a prototype that incorporates the new compound. Due to the lag between prototyping and market release, the products in my analysis are not yet mass-produced or available to consumers.

**Scientist Activities** I observe rich text data on scientists' work. Required for administrative purposes, researchers meticulously log their tasks and the duration of each activity. On average, scientists record 7.8 entries per week, totaling more than 1.6 million observations over my four year sample.

To transform this textual information into a meaningful quantitative metric, I separate the materials discovery process into three categories of tasks: idea generation, filtering, and experimentation. Idea generation encompasses activities related to developing potential compounds, such as reviewing the literature on existing materials or creating preliminary designs. Filtering tasks focus on selecting which compounds to advance, often involving the analysis of simulations or predicting material characteristics based on domain knowledge. Finally, experimentation tasks are dedicated to synthesizing new materials and conducting tests to evaluate their properties. Based on the materials science literature and discussions with the lab's scientists, these categories divide the discovery process into meaningful, high-level groups.

I employ a large language model—Claude 3.5 Sonnet—to classify scientists' activities into these categories (with a fourth for all other tasks). This enables me to quantify the amount of time scientists dedicate to each stage. I fine-tune the model using manually classified training data, improving its performance substantially. I validate my classification procedure using out of sample predictions and a survey of the lab's scientists, confirming that the model accurately categorizes research activities. Appendix B.5 provides further details on the text data, classification process, and validation.

**Scientist Characteristics** I also observe data on scientists' education, demographics, employment history, academic publications, and past discoveries. These are used as control variables and to evaluate treatment effect heterogeneity.

**Other R&D Inputs** Finally, I use information on the lab's input costs to construct a measure of R&D efficiency. This includes expenditures on scientist wages, lab equiment, and raw materials, as well as training and inference costs for the model.

### 3.2 Survey of Scientists

I supplement these data by conducting a survey of the lab's scientists. The survey has three objectives: first, to understand how researchers collaborate with the model and determine why some are more skilled at evaluating AI suggestions; second, to validate the task allocation measures; and third, to assess the tool's impact on scientists' job satisfaction and beliefs about artificial intelligence. I match respondents to the researchers in my panel.

I sent the 15-minute survey to all 1,018 scientists in my sample. To incentivize participation, it states that the results will inform the lab's plans regarding future AI use. I received 447 responses (44%). This response rate is relatively high—the median paper in a top economics journal has a response rate of 35% (Dutz et al., 2022) and for surveys of scientists it can be well below 10% (Hill and Stein, 2024; Myers et al., 2024). Appendix Table A8 reports the characteristics of respondents. They are representative in terms of educational background, material of focus, and past performance, but skew slightly younger and less experienced. Appendix Table A9 shows the number of responses to each survey question. While there is some attrition, more than two thirds of respondents answered all questions.

I fielded the survey in May and June of 2024, after all scientists had gained access to the model. Consequently, the results should be interpreted as descriptive. The survey instruments are provided in Appendix C.

### 3.3 Sample Selection and Summary Statistics

My panel covers the period between May 2020 and June 2024, including two years of pre-treatment observations and 25 months after the start of the experiment. I restrict the analysis to ever-treated scientists who remain at the firm during the entire period. Additionally, I remove new hires and the small number of researchers who switched teams or roles. Attrition rates are low and do not vary between treatment and control groups. I consider only scientists who focus primarily on materials discovery, excluding lab technicians, administrators, and managers. Using the task data, I verify that all researchers in my sample indeed perform functions related to materials discovery. The final sample includes 1,018 scientists across 221 teams.

Table 1 reports descriptive statistics for the researchers in my sample, including their age, education, tenure at the firm, material specialization, and innovative output. They are highly

educated, with more than 60% holding a PhD, and have worked at the firm for an average of 8.4 years. Scientists are divided roughly evenly between four material categories: biomaterials (including synthetics), ceramics and glasses, metals and alloys, and polymers. The typical scientist produces 0.56 new materials, 0.16 patent filings, and 0.20 product prototypes each year. Discovery rates vary somewhat by material type, with biomaterials having the highest rates and metals the lowest.

### 3.4 Research Design

The random assignment of research teams to adoption waves provides a favorable setting for identification. I therefore estimate simple two-way fixed effects specifications at the team level:

$$\text{Static:} \qquad y_{it} = \alpha_i + \gamma_t + \delta D_{i,t-l} + \varepsilon_{it} \tag{1}$$

$$\text{Event Study:} \qquad y_{it} = \alpha_i + \gamma_t + \sum_{k \in [\underline{k}, \bar{k}]} \delta_k D_{it-k} + \varepsilon_{it} \tag{2}$$

where $y_{it}$ is the inverse hyperbolic sine of the outcome of interest, $D_{it}$ is a treatment indicator, and $\alpha_i$ and $\gamma_t$ are team and month fixed effects. The static specification includes a lagged structure to capture the average treatment effect once the full impact of AI has been realized.

Randomization ensures strong ignorability, so under a stable unit treatment value assumption $\delta$ captures the average treatment effect. To confirm that teams were indeed randomly assigned to treatment groups, Table 1 reports balance tests for the three waves, showing no systematic differences. My primary specifications include no additional controls, but the results are robust to the addition of covariates. To estimate individual treatment effect heterogeneity, I run scientist-level versions of these specifications.[11]

Several papers note that ordinary least squares estimates of Equations (1) and (2) may be biased if treatment effects vary over time or across adoption cohorts. The results are similar using the unbiased estimators proposed by de Chaisemartin and D'Haultfœuille (2020), Callaway and Sant'Anna (2021), Sun and Abraham (2021), and Borusyak et al. (2024).

I conduct inference in two ways. In my main results, I report standard $t$-based confidence intervals, clustering at the team level. Following the econometrics literature on experiments (Athey and Imbens, 2017; Abadie et al., 2020), I also take a design-based approach and perform permutation tests. All findings are robust to the choice of inference strategy.[12]

[11] Because scientists within a team are treated simultaneously and have correlated outcomes, these individual effects are less well-identified. I therefore also assess treatment effect heterogeneoity at the team level. The results are similar but more muted, since teams display less variation in research productivity than individual scientists

[12] Results using randomization inference are reported in Appendix Table A4.

**Table 1.** Summary Statistics and Treatment Group Balance

| | Full Sample (All Periods) | Wave 1 (Pre-Treatment) | Wave 2 (Pre-Treatment) | Wave 3 (Pre-Treatment) | Normalized Difference |
|---|---|---|---|---|---|
| ***Scientist Characteristics*** | | | | | |
| Age (Years) | 45.78 | 45.75 | 45.88 | 45.60 | 0.04 |
| Tenure at Firm (Years) | 8.02 | 8.25 | 7.79 | 8.06 | 0.06 |
| Share Bachelors Degree | 0.06 | 0.07 | 0.04 | 0.05 | 0.06 |
| Share Masters Degree | 0.33 | 0.30 | 0.33 | 0.40 | 0.06 |
| Share Doctoral Degreee | 0.61 | 0.63 | 0.63 | 0.56 | 0.05 |
| Share Chemical Engineers | 0.22 | 0.21 | 0.23 | 0.19 | 0.06 |
| Share Chemists | 0.14 | 0.13 | 0.14 | 0.15 | 0.03 |
| Share Materials Scientists | 0.23 | 0.25 | 0.22 | 0.24 | 0.04 |
| Share Physicists | 0.10 | 0.07 | 0.11 | 0.15 | 0.06 |
| Share Other Fields | 0.31 | 0.34 | 0.30 | 0.26 | 0.05 |
| ***Material Specialization*** | | | | | |
| Share Biomaterials | 0.25 | 0.24 | 0.26 | 0.26 | 0.04 |
| Share Ceramics and Glasses | 0.19 | 0.19 | 0.19 | 0.21 | 0.05 |
| Share Metals and Alloys | 0.32 | 0.34 | 0.34 | 0.20 | 0.04 |
| Share Polymers | 0.24 | 0.22 | 0.21 | 0.33 | 0.04 |
| ***Innovative Output*** | | | | | |
| New Materials (Yearly) | 0.56 | 0.45 | 0.40 | 0.44 | 0.05 |
| Patent Filings (Yearly) | 0.16 | 0.14 | 0.09 | 0.14 | 0.06 |
| Product Prototypes (Yearly) | 0.20 | 0.17 | 0.12 | 0.17 | 0.04 |
| ***Sample Size*** | | | | | |
| Number of Teams | 221 | 89 | 91 | 41 | – |
| Scientists per Team | 4.61 | 4.53 | 4.60 | 4.78 | 0.03 |

*Notes:* The first column reports summary statistics for the full sample of scientists between May 2021 and June 2024. The middle three columns show pre-treatment means separately by adoption wave. The final column reports the maximum pairwise normalized difference between wave-specific means, calculated as: $\frac{|\bar{X}_1 - \bar{X}_2|}{\sqrt{(s_1^2 + s_2^2)/2}}$. The normalized differences are below 0.07, providing strong evidence of balance.

# 4 The Impact of AI on Scientific Discovery and Innovation

## 4.1 New Materials, Patent Filings, and Product Prototypes

I begin by presenting descriptive evidence of AI's impact on materials discovery, patenting, and product innovation. Figure 4 plots time series of the three outcomes for treated and untreated scientists, revealing a marked rise in new compounds and patent filings after AI-adoption. Ten to twelve months later, this is followed by an increase in product prototypes incorporating the discovered compounds.

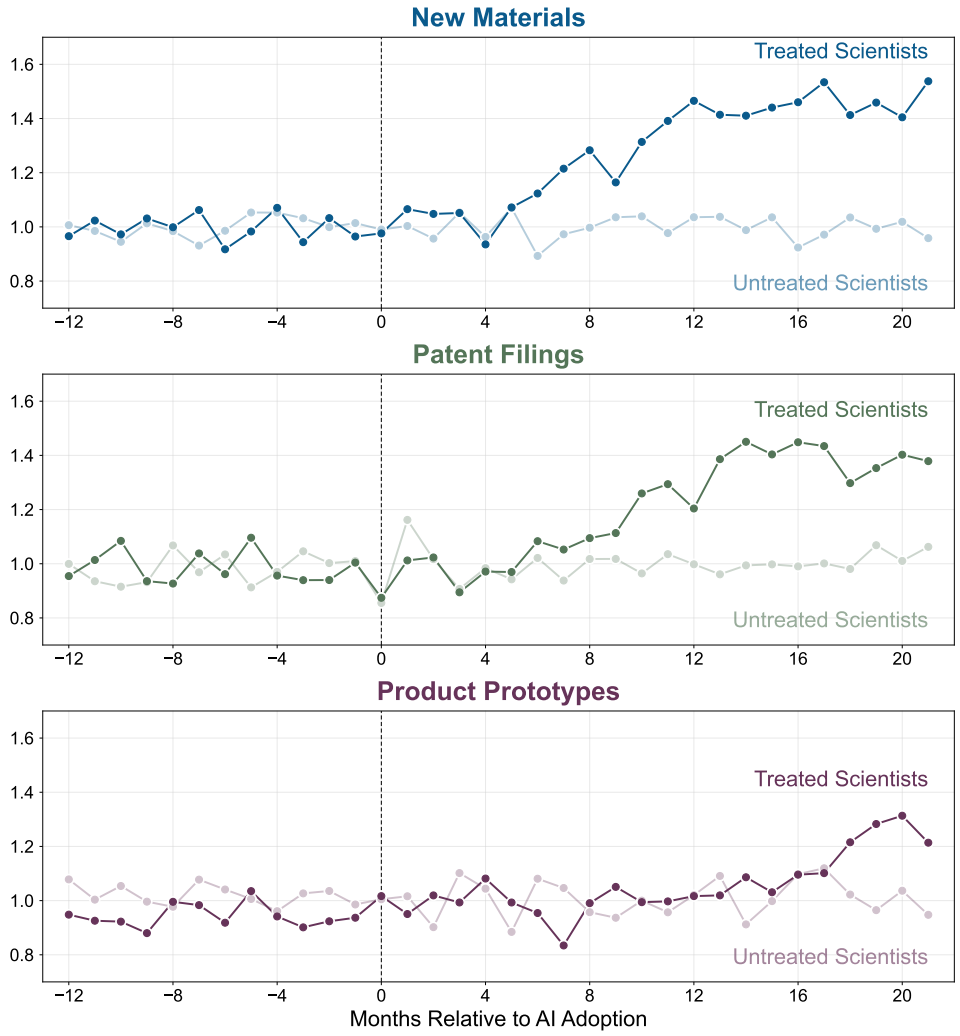



**Figure 4.** Time Series of Innovation Rates in Treatment and Control Groups

*Notes:* This figure plots monthly time series of new materials, patent filings, and product prototypes for treated and untreated scientists. In the pre-period, the "untreated" group includes scientists from the third wave (treated in month 12), while the "treated" group includes waves 1 and 2. To facilitate comparison, I normalize the levels of the variables so that they average 1 in the pre-period. This figure is in months relative to AI adoption. Appendix Figure **??** plots a time series of each outcome in calendar time, showing an equivalent pattern.

Next, I turn to the regression estimates. Figure 5, Panel A reports endline treatment effects for the last five months of the sample. On average, AI-assisted scientists discover 44% more materials, leading to a 39% increase in patent filings and a 17% rise in product prototypes. To investigate dynamics, Panel B plots event study estimates. The results show a similar pattern to the raw time series: the effects on materials discovery and patenting emerge after 5-6 months, while the impact on product innovation lags by more than a year. Both specifications include team and month fixed effects and I report 95% confidence intervals based on standard errors clustered at the team level. Appendix Tables A1–A6 show the robustness of these estimates to alternative specifications, finding nearly identical results.

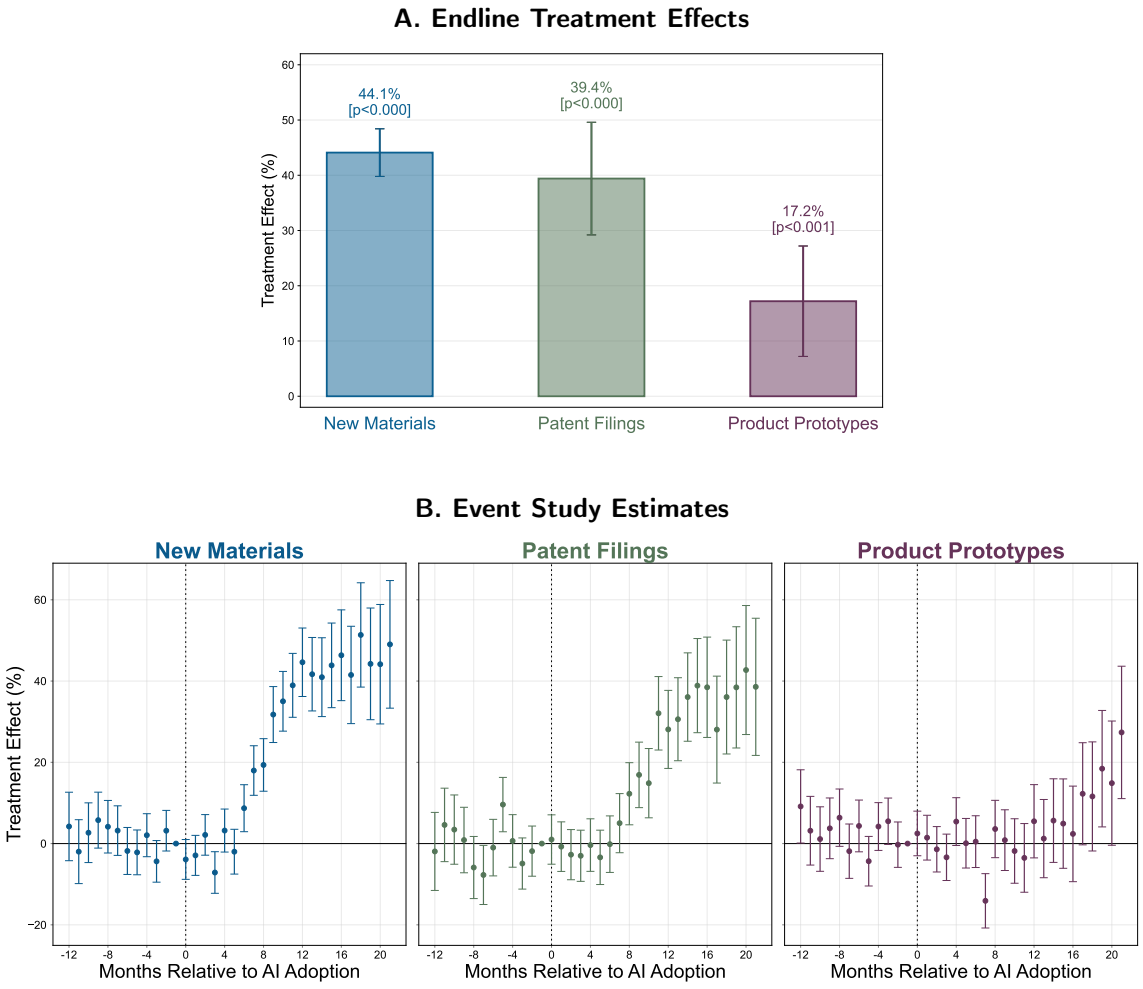



**Figure 5.** Impact of AI on Materials Discovery, Patent Filings, and Product Prototypes

*Notes:* This figure shows the impact of AI on new materials, patent filings, and new products. Panel A plots endline treatment effects for the last 5 months of the sample. Panel B present event study estimates for the three outcomes following the specification in Equation (2). Both specifications include team and month fixed effects and report 95% confidence intervals based on standard errors clustered at the team level. The estimates are converted to percentage terms based on pre-treatment means.

These effects are large. To put the increase in materials discovery in perspective, the lab's research output per scientist declined by 4% over the preceding five years. This was despite the introduction of several computational tools designed to aid scientists. AI therefore appears to be a different class of technology, with effects that are orders of magnitude larger than previous methods.

While still representing a substantial increase in innovation, the downstream impact on product prototypes is about half as large. This could reflect several factors. First, the lag between discovery and product development means that some new materials may have yet to be integrated into prototypes. Second, as I show in Section 4.3, AI increases the share of products that represent new lines rather than improvements to existing ones. The smaller effect could thus reflect a compositional shift toward more challenging inventions. Finally, prototyping may simply be a bottleneck, partially attenuating the impact of faster materials discovery.

I conduct several exercises testing the robustness of these findings. One scenario that would invalidate my research design is if teams within the firm race to make discoveries. In this case, AI would impact innovation rates for untreated scientists in the opposite direction, leading to upward bias in the estimated treatment effect. While time series evidence on discoveries in the treatment and control groups shows no signs of such spillovers (see Figure 4), I devise an identification strategy robust to the presence of racing. For each treated team, I construct a control group composed of untreated teams not working in the same subspecialty. I implement this design by estimating subspecialty-specific treatment effects that are aggregated into an average impact. The resulting estimates are nearly identical to the coefficients using the full sample, suggesting that racing dynamics are not a concern in my setting. Furthermore, R&D spending is similar between treated and control teams, showing that the effects are not driven by differential investment. Finally, the results do not reflect a compositional shift in the types of materials scientists focus on.

### 4.2 Material Quality

AI increases the number of new compounds. However, it could be the case that it simultaneously lowers material quality. Indeed, human science appears to exhibit such a speed-quality tradeoff (Hill and Stein, 2024). If so, my estimates would overstate the tool's impact. While the patent and product results help mitigate this concern, I use material properties to test quality directly. As described in Section 3, I construct quality indices based on the distance between scientists' target characteristics and compounds' observed properties.

Table 2 shows the impact of AI on my three quality measures. For atomic properties, the tool increases average quality by 13% and raises the proportion of top-decile materials by 1.7

percentage points (Columns 1-2). Large-scale characteristics exhibit a similar but slightly smaller effect (Columns 3-4). Columns (5) and (6) combine both sets of properties into an overall index, showing statistically significant improvements in average quality (9%) and the proportion of high-quality materials (1.5 pp).

These indices combine a number of characteristics that may vary in importance to the firm, making it difficult to interpret the magnitude of these estimates. However, the results suggest that AI-assisted discovery does not compromise material quality. Appendix B.2 provides details on the construction of the similarity measures.

**Table 2.** Impact of AI on Material Quality

| | *Atomic Properties Index* | | *Large Scale Properties Index* | | *Overall Quality Index* | |
|---|---|---|---|---|---|---|
| | Average (1) | Share Top 10% (2) | Average (3) | Share Top 10% (4) | Average (5) | Share Top 10% (6) |
| Access to AI | 0.066*** | 0.0017* | 0.034** | 0.0014** | 0.045*** | 0.0015** |
| | (0.032) | (0.0009) | (0.003) | (0.0008) | (0.004) | (0.0008) |
| Month Fixed Effects | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| Team Fixed Effects | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| Material Type Fixed Effects | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 | 221 | 221 | 221 |

*Notes:* This table presents the impact of AI access on three material quality metrics. For each metric, I report the average effect and the impact on the share in the top 10% of the distribution. Columns (1) and (2) present the results for atomic properties, columns (3) and (4) for large scale properties, and columns (5) and (6) for an overall index that combines the two. The construction of these measures is described in Appendix B. Standard errors in parentheses are clustered at the team level. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

### 4.3 Novelty

While AI accelerates the pace of innovation, the consequences hinge on the nature of these breakthroughs. Would they have occurred anyway, just at a later date? I present three pieces of evidence that suggest the answer is no. Instead, the tool engenders a shift toward more radical innovation, increasing novelty in all three stages of R&D.

I first measure the novelty of new materials themselves, following the chemical similarity approach described in Section 3. Shown in Table 3, Column (1), AI decreases average similarity by 0.2 standard deviations. Furthermore, it increases the share of highly distinct materials—defined as those in the bottom quartile of the similarity distribution—by 4 percentage points (Column 2). I corroborate these measurements with the survey of scientists. Consistent with my estimates, 73% of researchers report that the tool generates more novel designs than other methods.

Since the tool is trained on existing materials, one might have expected it to create structures that

closely resemble known compounds. The fact that it instead increases novelty can be interpreted in two ways. One possibility is that the model is simply adept at generalization, exploring new parts of the materials design space. The extent to which neural networks can generalize is an open question, but recent evidence suggests that such capabilities are possible (Zhang et al., 2024). Alternatively, this finding could primarily reflect human limitations in the absence of AI, with scientists adhering even more closely to familiar templates.

While chemical similarity captures a key aspect of scientific novelty, it is important to determine whether more original materials lead to more innovative technologies. To do so, I analyze the textual similarity of patent filings. As described in Section 3, I calculate two similarity metrics. The first is based on the full text of filings and the second on the share of new technical terms. Shown in Column (3) of Table 3, the tool boosts novelty on the first measure by 11%, shifting the average filing from the 48th to 42nd percentile of the similarity distribution. On the second measure, shown in Column (4), AI increases the share of new technical terms—a leading indicator of transformative technologies—by two percentage points (22%).

Finally, I study the tool's impact on the nature of product innovations. In the absence of AI, scientists focus primarily on improvements to existing products, with only 13% of prototypes representing new lines. As shown in Column (6) of Table 3, this share rises by 3 percentage points in the treatment group (18%). This suggests that the firm has a pipeline of product ideas, but a lack of viable materials represents a barrier to their creation. By relaxing this constraint, AI enables a shift toward more radical innovation.

A central concern with applying big data and machine learning to scientific discovery is the potential to amplify the "streetlight effect"—the tendency to search where it is easiest to look rather than where the best answer is likely to be. This worry stems from models being trained on existing knowledge, potentially directing search toward familiar but less promising areas (Khurana, 2023; Kim, 2023; Hoelzemann et al., 2024). In other words, AI might inefficiently favor exploitation over exploration. In materials science, this appears not to be the case. Instead, my findings show that the tool increases the novelty of discoveries, leading to more creative patents and more innovative products.

There are two important caveats to these results. First, they do not rule out the possibility that AI increases novelty within the neighborhood of what is known, but reduces the likelihood of truly revolutionary discoveries. This connects to a broader concern about the quantitative study of science: if progress is driven by outlier breakthroughs, empirical analyses may be misleading due to the inherent scarcity of right-tail discoveries (Nielsen and Qiu, 2022). Second, I do not observe the ultimate impact of the lab's inventions. I track patent filings, but lack data on citations or

subsequent innovations. Furthermore, the utility of the new products remains uncertain, as they are not yet available to consumers.

**Table 3.** Impact of AI on Novelty

| | Material Similarity (Mean) (1) | Material Similarity (Top 25%) (2) | Patent Similarity (Full Text) (3) | Patent Similarity (New Terms) (4) | Share New Product Lines (5) |
|---|---|---|---|---|---|
| Access to AI | 0.136*** | 0.0029* | 0.015** | 0.020*** | 0.020* |
| | (0.032) | (0.003) | (0.004) | (0.005) | (0.002) |
| Month Fixed Effects | ✓ | ✓ | ✓ | ✓ | ✓ |
| Team Fixed Effects | ✓ | ✓ | ✓ | ✓ | ✓ |
| Number of Scientists | 651 | 651 | 1,018 | 1,018 | 1,018 |
| Number of Teams | 145 | 145 | 221 | 221 | 221 |

*Notes:* Columns (1) and (2) presents the results for material novelty, which I measure using the similarity approach of De et al. (2016). This applies ony to the 54% of crystal structures in my sample. Column (1) shows average similarity and Column (2) shows the share in the top 25% of similarity based on a cutoff defined in the pre-period. Columns (3) and (4) report the estimates for patent novelty using the textual similarity metrics of Kelly et al. (2021) and Kalyani (2024), respectively. Finally, column (6) shows the impact on the share of product prototypes that are new lines (rather than improvements to existing lines). The construction of the novelty measures are described in Appendix B. Standard errors in parentheses are clustered at the team and month level. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

### 4.4 R&D Efficiency

Finally, I combine my estimates with data on input costs to calculate the tool's impact on R&D efficiency. Using number of product prototypes as the outcome, I define efficiency as:

$$\text{R\&D Efficiency} = \frac{\text{Product Prototypes}}{\text{Labor Costs} + \text{Other Variable Costs} + \text{Amortized Fixed Costs}}$$

Labor costs include salaries and benefits for the lab's scientists, technicians, and other staff, which are identical across treatment waves. Non-labor variable costs are higher for treated scientists, due to increased spending on testing, product development, and model inference. Importantly, fixed costs include expenditure on training the model, which I conservately amortize over a 5-year period. Depending on the specific set of costs included, I find that AI boosts efficiency by 13-15 percent.

# 5 Heterogeneity by Scientist Ability

AI substantially increases the average rate of materials discovery. However, I now document considerable heterogeneity in its effects across scientists. The tool disproportionately benefits researchers with high initial productivity, exacerbating inequality. Decomposing productivity into distinct skills, I show that differences in discernment—the ability to identify promising candidate compounds—explain nearly all of this heterogeneity.

## 5.1 The Impact of AI Across the Productivity Distribution

Figure 6, Panel A shows the distribution of materials discovery rates before and after the introduction of AI. The distribution shifts to the right and becomes substantially more right-skewed, suggesting that high ability scientists gain more from the tool. To test this systematically, I construct a measure of initial productivity based on materials discovered in the pre-treatment period. I control for material type and application to account for the possibility that some compounds are inherently easier to create. Additionally, as discussed in Section 3, all scientists in my sample work primarily in materials discovery roles, so variation in productivity does not reflect a different area of focus. The resulting metric is positively correlated with the ranking of scientists' graduate instituitons as well as tenure in the lab, suggesting that it indeed captures a notion of ability. Moreover, discovery rates are persistent over time, showing that they reflect skill rather than luck.

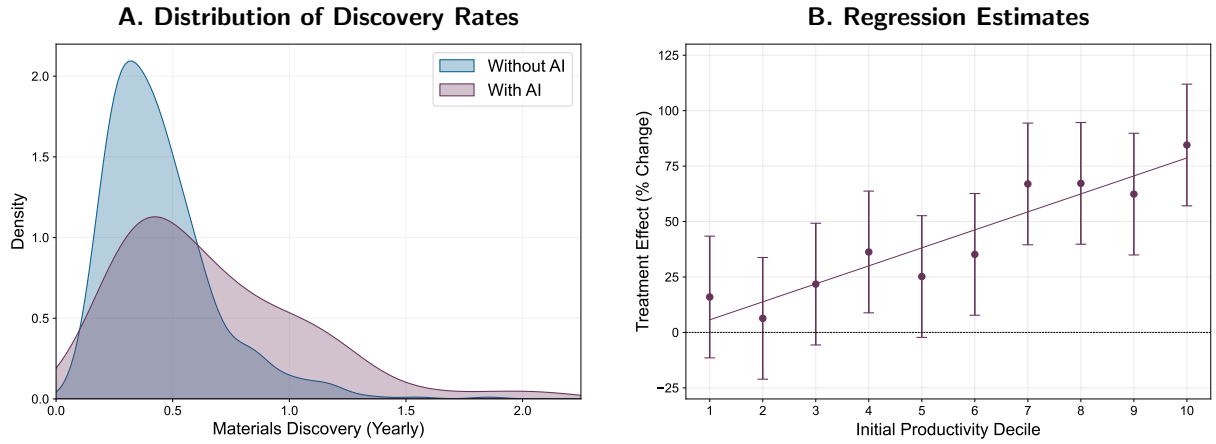



**Figure 6.** Impact on Materials Discovery by Initial Productivity

*Notes:* Panel A shows the distribution of yearly materials discovery rates for scientists with and without AI. Panel B shows AI treatment effects for each decile of initial productivity. These estimates come from interacting a treatment indicator with dummy variables for being in each decile. I report 95% confidence intervals clustered at the team level.

Figure 6, Panel B presents regression estimates, interacting treatment status with deciles of initial productivity. The bottom third of scientists see little benefit from the tool, while the output

of top scientists increases by 78%.[13] As a result, the ratio of 90:10 research performance more than doubles. The fact that the tool boosts inequality is in constrast to recent evidence on large language models (Brynjolfsson et al., 2023; Noy and Zhang, 2023; Peng et al., 2023), showing that the distributional consequences of AI depend on the context and type of technology. Appendix Figure A4 reports analogous results for patenting and product prototypes, showing a similar pattern for these downstream outcomes.

These results suggest that AI and scientific expertise are complements in the innovative process. The rest of the paper investigates the source of this complementarity.

## 5.2 Heterogeneity by Dimension of Skill

Why do highly productive scientists benefit more from AI? As described in Section 2, materials discovery involves three steps: idea generation, filtering, and experimentation. Thus, overall productivity is determined by scientists' varying abilities in each phase. I now show that skill in a single step—filtering—explains nearly all of the tool's heterogeneous impact.

### 5.2.1 Estimating Task-Specific Research Abilities

I begin by estimating each scientist's task-specific research ability in the pre-treatment period. Because the experimentation phase consists solely of routine tests, I focus on idea generation and filtering. The ideal experiment to identify these measures would assign a random set of scientists to design candidate materials and another to filter them. Lacking explicit randomization, I exploit the division of labor within teams. The set of scientists assigned to work on a given material—as well as the specific research tasks they perform—varies significantly across compounds. Combined with two key assumptions, this variation allows me to identify task-specific skills.

Let $\gamma_s^g$ and $\gamma_s^f$ represent scientist $s$'s skill in idea generation and filtering tasks, respectively. Suppose the probability that candidate material $m$ is viable is given by:

$$\mathbb{P}\left(\text{Viable}\right)_m = \frac{1}{|\,S^g\,|}\sum_{s\in S^g}\gamma_s^g + \frac{1}{|\,S^f\,|}\sum_{s\in S^f}\gamma_s^f + \theta' W_m + \varepsilon_m \tag{3}$$

where $S^g$ and $S^f$ are the sets of scientists that work on idea generation and filtering tasks for material $m$, respectively. This equation states that expected material viability reflects average skill in idea generation for scientists working on the design step, average skill in filtering for scientists working on the prioritization step, and material-specific controls, $W_m$. Variation in $S^g$ and $S^f$ across

[13] Appendix Figure A3 presents analogous estimates at the team level, showing a similar but more muted pattern.

compounds enables me to estimate $\gamma_s^g$ and $\gamma_s^f$ for each scientist.[14]

Two assumptions are critical in this design. First, it must be the case that $S^g$ and $S^f$ are orthogonal to $\varepsilon_m$, conditional on $W_m$. In other words, the set of scientists assigned to work on a particular material are unrelated to its latent viability. This assumption would be violated, for example, if researchers with low idea generation ability were assigned to materials that are easier to design, even after controlling for observables. Two features of my setting help mitigate this concern. First, scientists within a team are assigned to materials through a queue-based system, so material allocation is primarily determined by availability. Additionally, I observe detailed information on the characteristics of compounds, allowing me to include rich controls for material type and intended application. The second identifying assumption is that $\gamma_s^g$ and $\gamma_s^f$ are additively separable. This rules out match effects between scientists working on the same material.

I conduct several tests to validate my ability measure. First, I find that $\hat{\gamma}_s^f$ and $\hat{\gamma}_s^g$ are autocorrelated, suggesting that the estimates reflect underlying skill rather than chance. Second, I document a relationship between academic background and task-specific ability. For a subset of scientists, I observe their journal publications and doctoral dissertations. Scientists who study topics related to a specific research task tend to be especially skilled in that area. For instance, a scientist who developed a novel simulation technique for predicting material properties is more likely to have an advantage in filtering tasks. Third, I observe that researchers are more likely to specialize in tasks where they have a comparative advantage. Finally, I corroborate the estimates with survey data. I ask each scientist to rate their skills in idea generation and filtering on a 1-10 scale and compare their abilities to their peers. These self-assessments align with my empirical findings, in both absolute and relative terms. Indeed, all the results are directionally consistent if I simply use researchers' self-reports rather than estimated ability.

#### 5.2.2 Correlation Between Dimensions of Skill

Figure 7 plots the correlation between scientists' skill in idea generation and discernment. The two measures are positively correlated ($r = 0.42,\ p < 0.00$). This suggests that scientists possess some form of underlying expertise that makes them productive in both sets of tasks. However, the correlation is well below one, revealing a potential role for comparative advantage and specialization. This underscores the importance of moving beyond a one-dimensional notion of "skill-bias" to examine the specific abilities that are complemented by AI.

[14] Given its high-dimensional nature, I estimate Equation (3) using an empirical Bayes approach (Chetty et al., 2014; Kline et al., 2022). Specifically, I assume that the underlying distribution task-specific ability is normal and shrink the estimated fixed effects toward the mean of this distribution.

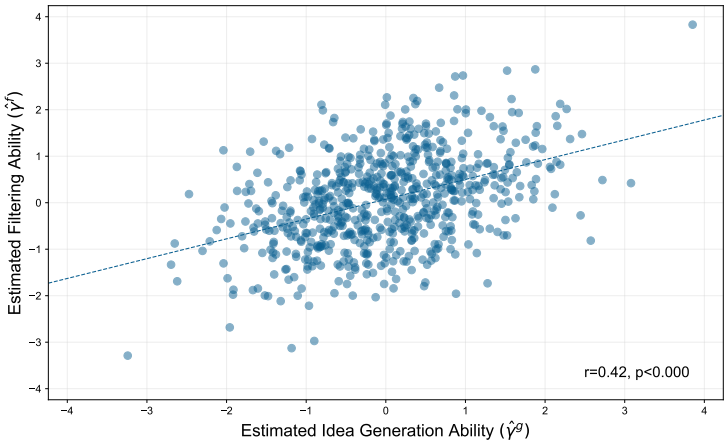



**Figure 7.** Correlation Between Research Skills

*Notes:* This figure the relationship between scientists' skill in idea generation and filtering, plotting $\hat{\gamma}_s^g$ against $\hat{\gamma}_s^f$. These measures are based on the fixed effects specification in Equation 3. The correlation coefficient is 0.42 (p<0.00).

### 5.2.3 The Impact of AI by Dimension of Skill

Armed with estimates of task-specific research ability, I examine which skills drive the heterogeneous impact of AI. To do so, I estimate the following regression at the scientist level:

$$y_{st} = \beta_1 D_{st} + \beta_2 \tilde{\gamma}_s^g + \beta_3 \hat{\gamma}_s^f + \beta_4 D_{st} \times \hat{\gamma}_s^g + \beta_5 D_{st} \times \hat{\gamma}_s^f + \varepsilon_{st} \tag{4}$$

where $y_{st}$ is the number of materials discovered by scientist $s$ in month $t$, $D_{st}$ is a treatment indicator, and $\hat{\gamma}_s^g$ and $\hat{\gamma}_s^f$ are estimated research skill in idea generation and filtering tasks, respectively. These measures are normalized to have mean zero and standard deviation one. The coeffients of interest are $\beta_4$ and $\beta_5$, capturing the differential impact of AI by task-specific skill.

The results are reported in Table 4. The coefficients on both interaction terms are positive and significant, but filtering ability has a substantially larger effect. A one standard deviation increase in $\hat{\gamma}^f$ corresponds to a 14.8 percentage point rise in the AI treatment effect. Meanwhile, an identical change in $\hat{\gamma}^g$ yields only a 3.5 percentage point increase. Consequently, differences in filtering ability explain more than 80% of the tool's heterogeneous impact by initial productivity.

These findings demonstrate the central role of filtering in explaining AI's disparate effects across scientists. In the next section, I explore why this is the case.

**Table 4.** The Impact of AI by Dimension of Research Ability

| | IHS Discovered Materials (1) | IHS Discovered Materials (2) | IHS Discovered Materials (3) |
|---|---|---|---|
| Access to AI | 0.0365*** | 0.0322*** | 0.0280*** |
| | (0.045) | (0.078) | (0.112) |
| $\hat{\gamma}^g$ | 0.2180*** | 0.2200*** | 0.2230*** |
| | (0.054) | (0.087) | (0.120) |
| $\hat{\gamma}^f$ | 0.2980*** | 0.3010*** | 0.3050*** |
| | (0.056) | (0.089) | (0.123) |
| Access to AI $\times\hat{\gamma}^g$ | 0.0001*** | 0.0001** | 0.0001** |
| | (0.0006) | (0.0010) | (0.0013) |
| Access to AI $\times\hat{\gamma}^f$ | 0.0061*** | 0.0052** | 0.0051** |
| | (0.0006) | (0.0011) | (0.0014) |
| Month Fixed Effects | ✓ | ✓ | ✓ |
| Material Type Fixed Effects | | ✓ | |
| Application Fixed Effects | | ✓ | |
| Material Type $\times$ Application Fixed Effects | | | ✓ |
| Number of Scientists | 845 | 845 | 845 |

*Notes:* This table reports heterogeneous treatment effects by scientists' abilities in filtering and idea generation, $\hat{\gamma}^f$ and $\hat{\gamma}^g$. These estimates come from the fixed effects specification in Equation (3). They are estimated in the pre-period and are thus constant for each scientist. Column (1) includes only time fixed effects, Column (2) adds material type and application fixed effects, and Column (3) instead includes material type by application fixed effects. Standard errors in parentheses are clustered at the scientist level. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

# 6 Tasks, Expertise, and Scientist-AI Collaboration

To summarize, I have documented three facts. First, AI substantially increases the average rate of materials discovery. Second, it disproportionately benefits researchers with high initial productivity. Third, this heterogeneity is driven almost entirely by differences in discernment ability. To understand the mechanisms behind these results, I investigate the dynamics of the human-AI collaboration.

I begin by developing a simple model of materials discovery, embedding research tasks in a canonical prioritized search framework. The model clarifies AI's role in accelerating invention and provides testable predictions for the allocation of research tasks and the changing returns to skill. Furthermore, it shows how organizational adaptation—in the form of hiring and firing practices—can amplify the tool's impact. Taking the model to the data, I confirm each of its key predictions.

I show that AI automates a majority of idea generation tasks, reallocating researchers to the new task of filtering model-produced candidate compounds. Scientists skilled in discernment learn to prioritize promising AI suggestions, while others waste significant resources testing false positives. The resulting gap in discovery rates explains the tool's heterogeneous impact. Survey evidence shows that these differences in evaluation ability are driven by domain knowledge. In the final month of my sample—excluded from the primary analysis—the firm changed its hiring and firing practices. Consistent with the theory, this resulted in a greater proportion of skilled evaluators

## 6.1 A Simple Model of Materials Discovery

**Set-up** Following Agrawal et al. (2023), I conceptualize materials discovery as a prioritized search problem. The research process requires three steps:

1. **Idea Generation:** Generate a set of candidate materials $\mathcal{M} = \{m_1, \ldots, m_M\}$. Each material has binary quality $\theta_m \in \{0, 1\}$, which depends on research inputs but is unobserved by scientists. Let $\bar{\theta} = \sum_{m=1}^{M} \theta_m$ be the share of high-quality materials.

2. **Filtering:** Evaluate candidate materials and rank them in descending order of predicted quality. Predictions improve with filtering, bringing the ranking $r : \mathcal{M} \to \{1, ..., M\}$ closer to the true ordering.

3. **Experimentation:** Conduct costly tests to reveal candidate materials' true quality. Each test imposes cost $c$ regardless of its result. Optimal search then takes a simple form: perform tests in the sequence implied by $r$, continuing until the cost of further search exceeds the

expected benefit (Weitzman, 1979; Agrawal et al., 2023). The discovery of a high-quality material gives payoff 1.

Scientists are endowed with a unit of labor and possess heterogeneous skills in idea generation and filtering tasks, denoted $\gamma^g$ and $\gamma^f$. Production in each stage proceeds as follows. Candidate materials are produced by combining a continuum of idea generation tasks $g(i)$. The share of high-quality candidates takes the following form:

$$\bar{\theta} = B_g(\sigma) \left( \int_0^1 g(i)^{\frac{\sigma-1}{\sigma}} di \right)^{\frac{\sigma}{\sigma-1}}$$

where $\sigma \in \mathbb{R}^+$ is the elasticity of substitution between tasks and $B_g(\sigma)$ is a normalizing constant. Idea generation tasks in the interval $[0, \tilde{I}]$ are automatable and are produced solely with AI. The remainder can be produced only with scientist labor $\ell$. Accordingly, the production function for task $i$ is:

$$g(i) = \begin{cases} a(i) & \text{if } i < \tilde{I} \\ \gamma^g \ell(i) & \text{if } i \in [\tilde{I}, 1] \end{cases}$$

Given a set of $M$ candidate materials—out of which $M\bar{\theta}$ are high-quality—scientists construct a ranking $r : \mathcal{M} \to \{1, ..., M\}$ based on their predicted quality. Let $p(k)$ be the probability that a material at position $k$ in the ranking of candidates is viable. Scientists test every material such that $p(k) \geq c$. I define the accuracy of the ranking, $R(c)$, as the share of high-quality materials that clear the testing threshold. This is a function of $c$ and ability-adjusted scientist labor allocated to filtering tasks. However, the use of AI for idea generation makes filtering more difficult, creating new filtering tasks:

$$R = \frac{B_f(\sigma) \left( \int_0^{1+\tilde{I}} f(i)^{\frac{\sigma-1}{\sigma}} di \right)^{\frac{\sigma}{\sigma-1}}}{c}$$

where $B_f$ is a normalizing constant. The production function for filtering task $i$ is $f(i) = \gamma^f \ell(i)$.

Figure 8, Panel A shows how $p(k)$ depends on filtering. With no filtering, tests are conducted at random, resulting in the flat curve $p(k) = \bar{\theta}$. Perfect filtering, in contrast, produces a step function, with all viable materials tested first. Intermediate filtering yields a curve between these extremes. I call $p(k)$ the "discovery curve," as it fully pins down the expected number of discovered compounds.

The expected number of discovered materials is then:

$$E\,(\text{Discoveries}) = \sum_{k:\, p(k) \geq c} \theta_k = M\bar{\theta}R(c)$$

**Visualizing the Impact of AI** In this framework, AI could impact the discovery process through two channels. First, the partial automation of compound design may affect the average quality of candidates, changing the area under the discovery curve. Second, AI-generated candidates may prove differentially challenging to evaluate, shifting the curve's slope. Figure 8, Panel B illustrates one potential scenario where AI increases $\bar{\theta}$ but makes candidates more difficulty to evaluate. Due to these competing forces, the net effect on the number of tests and the expected number of discovered compounds is ambiguous.

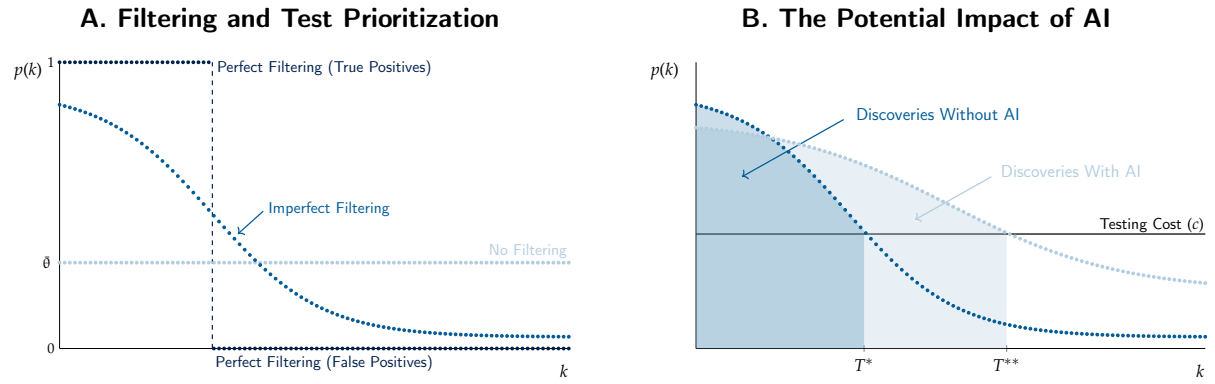



**Figure 8.** Materials Discovery as Prioritized Search

*Notes:* This figure depicts the materials discovery process as a prioritized search problem. Panel A shows the probability that a material at position $t$ is viable. The light blue line represents no filtering, with a constant discovery rate. The dark blue line illustrates perfect filtering, with all viable materials tested first. The medium blue line shows imperfect filtering. Panel B illustrates optimal search. Without AI, tests continue until $T^*$, with expected discoveries in the dark blue shaded region. AI increases the share of viable materials, but makes filtering harder. The curve flattens, and the optimal number of tested compounds rises to $T^{**} > T^*$. Expected discoveries are shown by the light blue shaded region.

**Model Predictions** The framework provides testable predictions for how AI will impact the research process. Let $\ell^g$ and $\ell^f$ be scientist labor allocated to idea generation and filtering tasks, respectively. Then, the model implies the following three propostions about how an increase in $\tilde{I}$, the share of automatable idea generation tasks, will impact the equilibrium.

**Proposition 1** (Task Reallocation). $\frac{\partial \ell^f}{\partial \tilde{I}} > 0$ *and* $\frac{\partial \ell^g}{\partial \tilde{I}} < 0$. *In other words, scientists reallocate labor from idea generation to filtering tasks after the introduction of AI.*

PROOF. See Appendix D. □

**Proposition 2** (Comparative Advantage and Reallocation). *Let* $\Gamma^f \equiv \frac{\gamma^f}{\gamma^g}$. *Then,* $\frac{\partial \ell^f}{\partial \tilde{I} \partial \Gamma^f} \geq 0$ *and* $\frac{\partial \ell^f}{\partial \tilde{I} \partial \Gamma^f} \leq 0$. *In other words, the reallocation effect is increasing in scientists' comparative advantage in discernment.*

PROOF. See Appendix D. □

The intuition for Propositions 1 and 2 is straightforward. AI automates a fraction of idea generation tasks, but creates new filtering tasks that can only be performed by scientists. It is then optimal for scientists to reallocate effort from idea generation to filtering tasks, leading to a decrease in $\ell^g$ and an increase in $\ell^f$. Because scientists are allocate labor to tasks according to their comparative advantage, this shift in tasks will be stronger for scientists with a comparative advantage in filtering.

**Proposition 3** (Returns to Skill). $\frac{\partial Y}{\partial \bar{I} \partial \gamma^f} > \frac{\partial Y}{\partial \bar{I} \partial \gamma^g}$. *In other words, automating idea generation tasks makes the returns to filtering ability relatively larger.*

PROOF. See Appendix D. □

The set of tasks performed by scientists becomes increasingly concentrated on filtering, increasing the importance of ability in these tasks. This explains the finding in Section 5.2 that AI was disproportionately beneficial to scientists skilled in filtering. Importantly, this result implies that it would boost productivity for the lab to alter their hiring and firing practices to favor scientists especially skilled in evaluation.

### 6.2 Automation, Task Creation, and Reallocation

Proposition 1 predicts that scientists will be reallocated from idea generation to filtering tasks after the introduction of AI. To test this empirically, Figure 9, Panel A plots the share of research hours dedicated to idea generation, filtering, and experimentation tasks, revealing a dramatic reorganization of the discovery process. These measures come from logs of scientist activities, employing the text classification procedure described in Section 3.

Without AI, scientists allocate 39% of their time to idea generation tasks. This drops to less than 16% after the model's introduction. In contrast, while filtering tasks initially take up 23% of research hours, they consume 40% by the end of the sample. Finally, the fraction of time dedicated to experimentation tasks increases from 37 to 44 percent, indicating that AI increases the number of tested compounds. Appendix Figure A2 reports event study estimates for these task shares, showing an identical pattern.

Proposition 2 predicts a stronger reallocation effect for scientists with a comparative advantage in evaluation. Panel B illustrates the change in task composition for scientists in the top and bottom quartiles of $\tilde{\Gamma}_s^f$. While all researchers significantly adjust their time allocation, those especially skilled in discernment display a 46% larger shift. Additionally, due to the complementarity between AI and evaluation ability, these scientists see a smaller increase in time spent testing materials.

In the task framework, it matters greatly whether scientists are reallocated to new evaluation tasks, or simply allocate more effort to the same set of tasks as before. Panel C shows the impact of

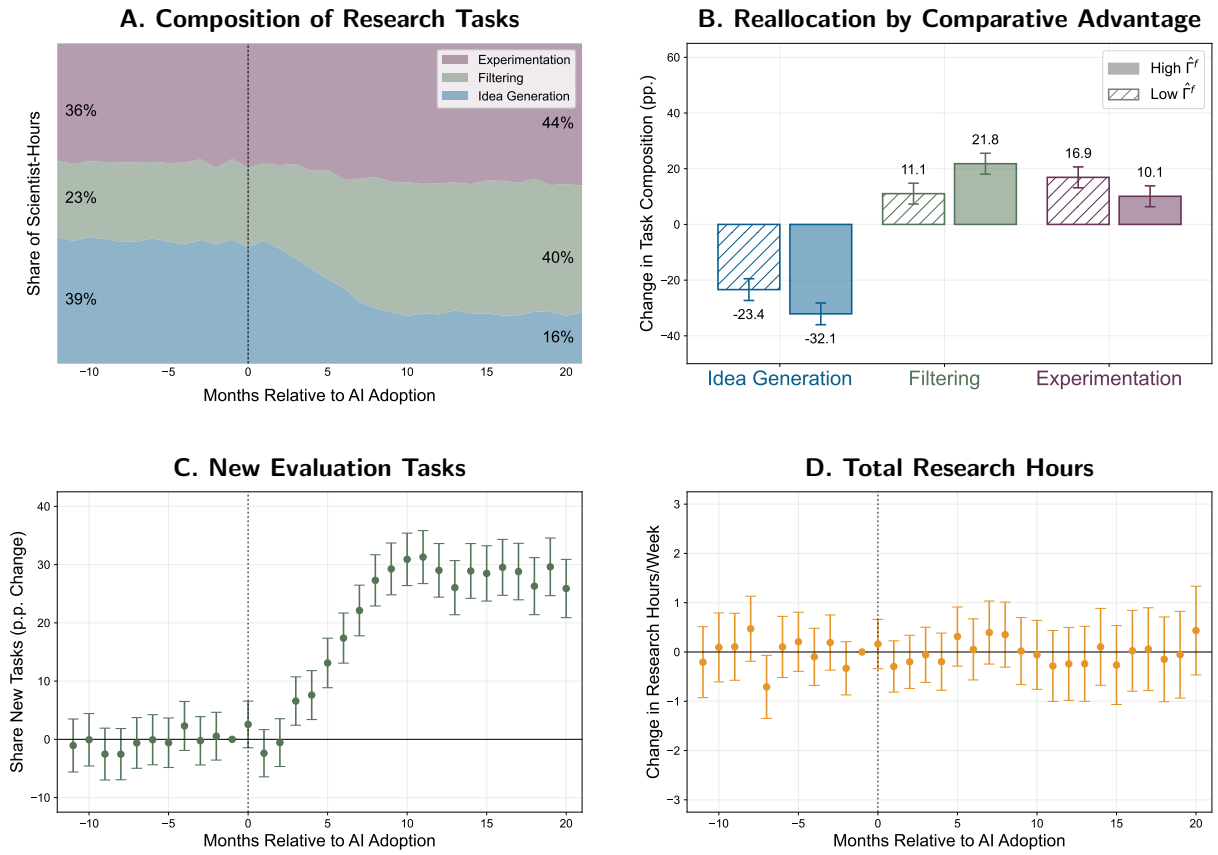



**Figure 9.** Impact of AI on Research Tasks

*Notes:* Panel A shows the share of scientists' research hours dedicated to idea generation (in blue), filtering (in green), and experimentation (in purple). The shares are normalized to exclude tasks not in these three categories. The x-axis shows months relative to the adoption of AI. The shares come from the classification procedure described in Section 3. Panel B shows the percentage point change in task allocation for scientists in the bottom and top quartiles of comparative advantage in filtering tasks. These measures are estimated using the fixed effects approach described in Section 5.2. The bars include 95% confidence intervals based on standard errors clustered at the scientist-level. Panel C shows the impact of AI on the share of filtering tasks that were not performed in the pre-treatment period. I calculate these measures using the scientist activities data. Panel D plots the effect of the tool on the total number of hours scientists spend each week on either idea generation, filtering, and experimentation tasks.

AI on the share of evaluation tasks that represent new activities, revealing a large and statistically significant increase. These results are based on the measures of new tasks described in Section 3.

I corroborate this evidence using the survey of scientists. Consistent with the task allocation measures, scientists report initially allocating 36% of their time to idea generation, 26% to filtering, and 42% to experimentation. After the introduction of AI, these shares become 13%, 35%, and 47%, respectively. Matching survey responses to the empirical results, I confirm that the shift from idea generation to filtering tasks is increasing in $\tilde{\gamma}_s^f / \tilde{\gamma}_s^g$. Moreover, scientists report that their process for evaluating AI-generated compounds is substantially different than traditional approaches, validating the observed rise in new tasks.

These results provide granular evidence on automation, task creation, and reallocation in science. AI automates 57% of design tasks, while scientists are reallocated to the new task of evaluating model-generated compounds. AI is thus labor-replacing in the specific acitivity of producing potential materials, but labor-augmenting in the broader discovery process due to task creation. Indeed, Panel D shows that scientists' total research hours were unchanged after the introduction of AI, revealing that demand for scientist labor remained high. Moreover, consistent with the theory, the relative magnitudes of these effects depend on scientists' comparative advantage. While the equilibrium impacts on employment and earnings are beyond the scope of this paper, my findings highlight the importance of considering new tasks when assessing the implications of AI for workers.

## 6.3 The Central Role of Discernment

### 6.3.1 The Empirical Discovery Curve

Consistent with the theory, I have shown that AI partially automates compound design, reallocating scientist labor to evaluation tasks. The resulting impact on materials discovery depends on scientists' effectiveness in these new tasks. In my framework, this is reflected in the "discovery curve"—the probability of finding a viable material at each position in the expected quality ranking. Leveraging the granularity of my data, I construct an empirical analog of this object: the share of viable materials at each position in the sequence of tested compounds.[15]

Figure 10, Panel A plots the empirical discovery curve before and after the introduction of AI, revealing a shift along three dimensions. First, the tool boosts the overall share of viable compounds, $\bar{\theta}$, captured by the increased area under the curve. Second, AI-generated compounds prove more difficult to evaluate, evidenced by the shallower slope in the treatment group. As I show in Section 6.3.2, this reflects the challenge of evaluating compounds scientists did not create. Third, the combination of these effects results in a greater number of materials tested overall.

Panels B and C compare post-treatment discovery curves for scientists in the top and bottom quartiles of discernment skill, revealing stark disparities in the ability to prioritize AI-generated compounds. The curve is essentially flat for scientists in the bottom quartile: their ranking of candidates is no better than random. In contrast, scientists in the top quartile learn to effectively identify promising AI suggestions. Their curve is also flat in the first five months after the tool's introduction. However, it becomes increasingly steep over the post-treatment period, reflecting learning.

[15] To create a curve that aggregates across many types of materials, I plot discovery rates normalized to the average viability of each material type.

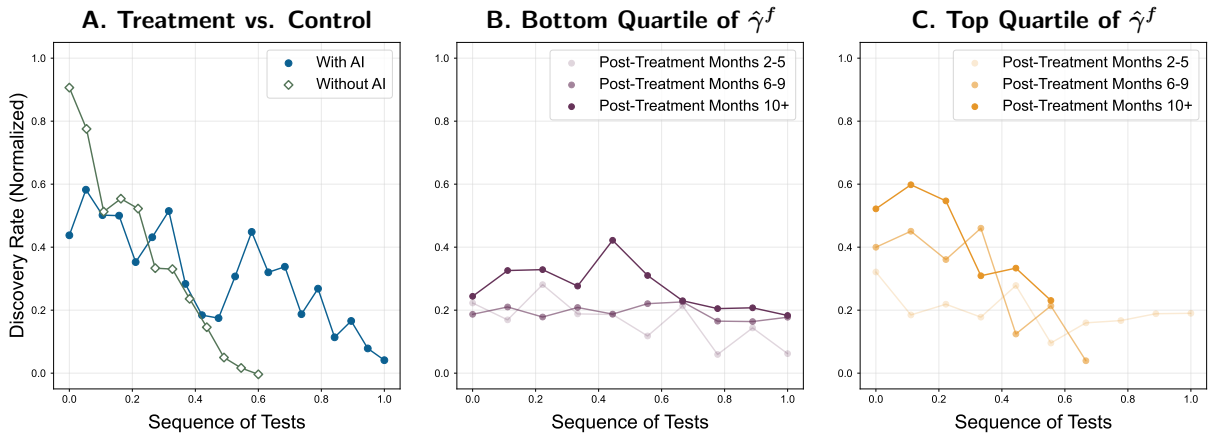



**Figure 10.** The Empirical Discovery Curve

*Notes:* This figure plots the empirical discovery curve, defined as the share of viable materials at each position in the sequence of tested compounds. To aggregate across different materials type, I create normalized discovery rates based on the average viability of each material category. Panel A shows the discovery curve for treated and control scientists. Panel B plots the curve for scientists in the bottom quartile of discernment ability, separated into three post-treatment periods: months 2-5, months 6-9, and months 10+. Panel B shows the curve for scientists in the top quartile of discernment ability over the same time periods. The estimates for discernment ability come from the fixed effects specification described in Section 5.2.

Due to these differences in prioritization, top researchers expend significantly less resources testing false positives, consistent with the task measures in the previous section. These results rationalize the central role of discernment ability in explaining the heterogeneous impact of AI.

### 6.3.2 Domain Knowledge and Discernment Ability

Why are some scientists so much better at evaluating model-generated compounds? To investigate this question, I turn to the survey of the lab's researchers. I ask scientists three questions about their evaluation process:

**Q1:** Compared to previous methods, how would you rate the difficulty of evaluating AI-generated candidate materials (much easier, somewhat easier, about the same, somewhat harder, much harder)?

**Q2:** How frequently can you identify AI-suggested candidate compounds as false positives without synthesizing the material (never/rarely/sometimes/often)?

**Q3:** On a scale of 1–10, how useful are each of the following in evaluating AI-suggested candidate materials (scientific training, experience with similar materials, intuition or gut feeling, and experience with similar tools)?

Consistent with my empirical results, 88% of scientists find AI-generated compounds more chal-

lenging to evaluate. The reason is simple: designing a material provides information about its quality. However, this increase in difficulty is not uniform across scientists. Compared to the bottom quartile, those in the top quartile of discernment ability are nearly twice as likely to report frequently ruling out false positives without testing (62% vs. 34%, $p < 0.00$).

This disparity suggests that top scientists possess some form of knowledge that allows them to effectively assess candidate materials. Figure 11 investigates four potential sources of this expertise. Panels A and B show that researchers in the top half of filtering ability place greater value on their scientific training and experience with similar materials when evaluating AI suggestions. The utility of "intuition or gut feeling" — a proxy for tacit knowledge — is also positively correlated with filtering skill (Panel C). In contrast, familiarity with similar AI tools does not explain the observed differences, as all scientists report minimal prior exposure (Panel D).

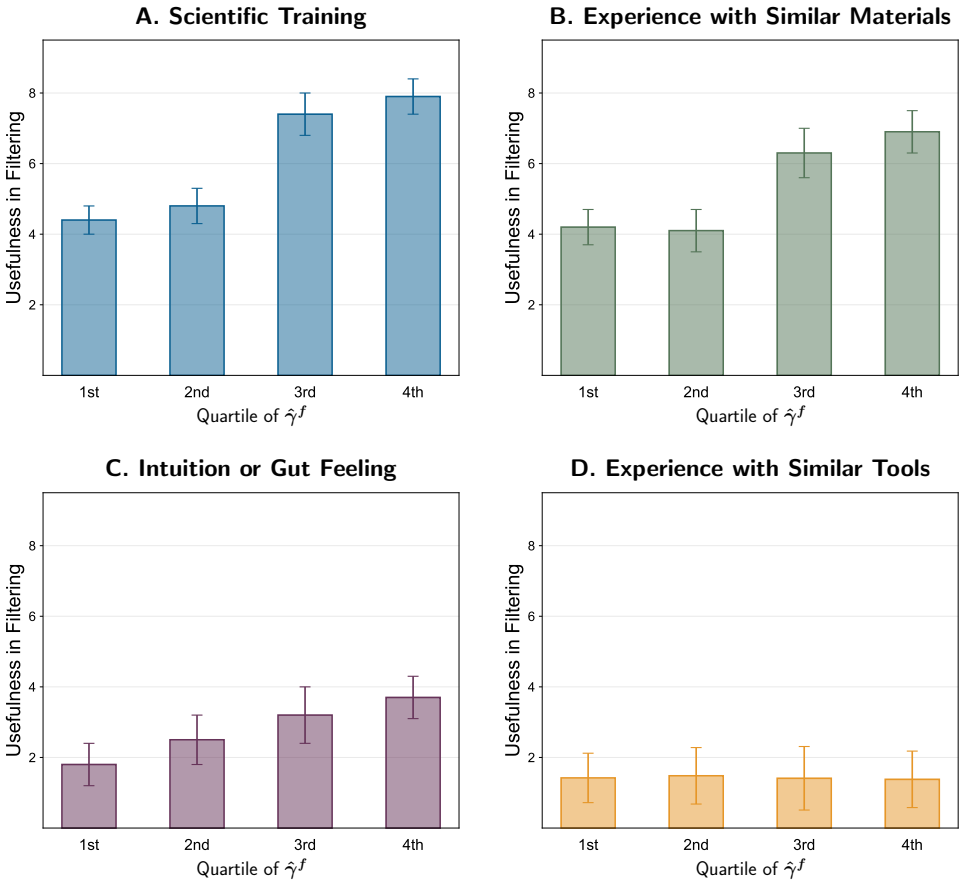



**Figure 11.** The Importance of Domain Knowledge in Discernment Ability

*Notes:* This figure shows the usefullness of different forms of expertise for evaluating AI-generated candidate materials. The results are reported on a 1-10 scale, separated by quartile of discernment ability. The top left panel presents the results for scientific training, the top right panel presents the results for experience with similar materials, the bottom left panel presents the results for intuition or gut feeling, and the bottom right panel presents the results for experience with similar tools. The bars include 95% confidence intervals. The survey instruments are provided in Appendix C.

These results demonstrate the importance of domain knowledge in evaluating AI suggestions. From a machine learning perspective, this shows that top scientists observe certain features of the materials design problem not captured by the model. Consequently, integrating human feedback into algorithmic predictions may be a promising path forward for scientific discovery (Hassabis, 2022; Alur et al., 2023, 2024). From an economic perspective, these findings highlight the complementarity between algorithms and human expertise in the innovative process. In particular, they emphasize the growing importance of a new research skill—evaluating model suggestions—that augments AI technologies.

Some have speculated that big data and machine learning will render domain knowledge obsolete (Anderson, 2008; Klein et al., 2017; Gennatas et al., 2020). In the context of materials science, this appears not to be the case. Instead, only researchers with sufficient expertise can harness the power of the technology. The fact that the tool is ineffective without skilled scientists suggests that demand for human researchers may remain strong, even as AI transforms scientific discovery.

### 6.4 Organizational Adaptation and Longer-Run Effects

Proposition 3 provides a channel through which organizational adaptation can amplify the tool's impact, leading to greater productivity gains in the long run. AI changes the returns to specific skills, increasing the value of discernment while reducing the importance of idea generation. Therefore, adjusting hiring and firing practices to prioritize researchers with strong discernment skills implies significant productivity gains.

In the final month of my sample—excluded from the primary analysis—the firm restructured its research teams, hiring a number of scientists and firing or reassigning several existing employees. While I do not observe the abilities of the new hires, the researchers who were let go were significantly more likely to have low filtering ability. Due to to these and other adaptations, it is possible that my estimates will underestimate the tool's longer-run impact.

## 7 Scientist Wellbeing and Beliefs About AI

AI substantially changes the materials discovery process. Using the survey, I explore how this impacts scientists' job satisfaction and beliefs about artificial intellgence. Beyond the direct welfare implications, these results shed light on AI's potential to shape who becomes a scientist, the fields they select into, and the skills they invest in.

### 7.1 Job Satisfaction

AI could affect scientists' job satisfaction in contrasting ways. It might boost morale by enhancing capabilities and increasing the rate of scientific discovery. Alternatively, it could make the work less enjoyable by shifting focus to less engaging tasks. To investigate the relative importance of these channels, I elicit changes in job satisfaction along three dimensions: those due to productivity shifts, those resulting from task reallocation, and the overall impact.

Figure 12, Panel A shows the results on a -10 to 10 scale, grouped by quartile of initial productivity. Two countervailing trends emerge: a mostly positive effect from increased productivity and a negative impact from task changes. The task reallocation effect is consistently negative across quartiles, ranging from -4.1 to -4.8. Scientists in the top half of ability experience enough productivity-driven satisfaction to offset their decreased task enjoyment, yielding a positive net effect. In contrast, the bottom half see a decline in overall satisfaction, with the first quartile experiencing a marked decrease.

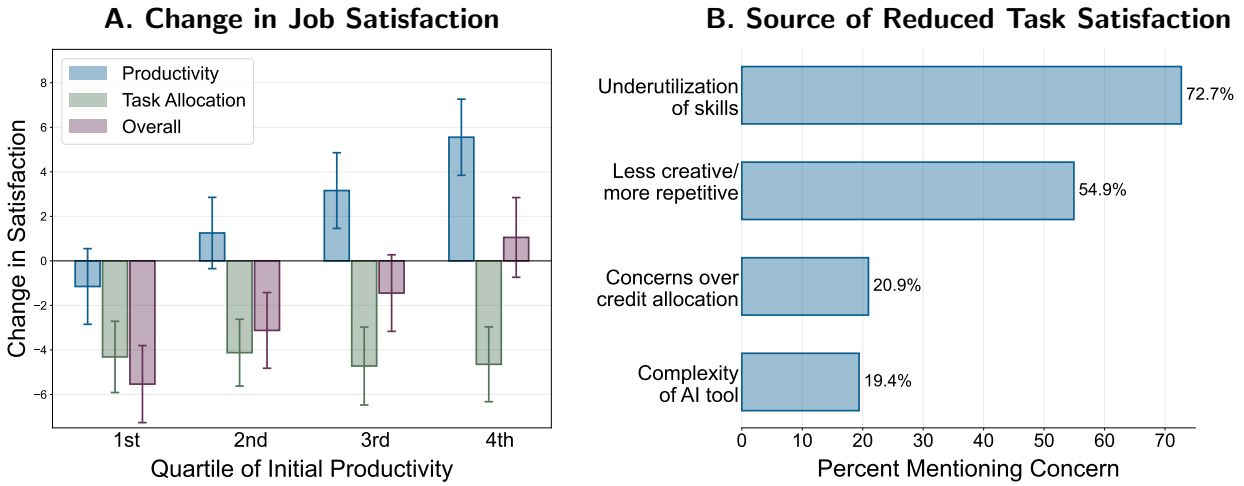



**Figure 12.** Impact of AI on Job Satisfaction

*Notes:* This figure shows the impact of AI on scientists' job satisfaction. Panel A displays changes in job satisfaction across quartiles of initial productivity, along with 95% confidence intervals. I report three measures: changes in satisfaction due to shifts in productivity (blue), changes in satisfaction due to shifts in task allocation (green), and overall changes in satisfaction (purple). Change in satisfaction is on a -10 to 10 scale, where negative values indicate decreased satisfaction, zero indicates no effect, and positive values indicate increased satisfaction. Panel B presents the primary sources of reduced task satisfaction. The x-axis shows the percentage of respondents mentioning each concern. The top four concerns are listed: underutilization of skills, less creative/more repetitive work, concerns over credit allocation, and complexity of the AI tool. The relevant survey questions are provided in Appendix C (questions 8-12).

The responses also highlight how organizational practices shape the welfare effects of AI. Scientists care not only about their own productivity, but their performance relative to their peers (Card et al., 2012). Consequently, despite seeing a small gain in research output (see Figure 6), scientists in the bottom quartile experience declining satisfaction with their productivity. This aligns

with the firm's promotion practices, as 83% of respondents report that advancement decisions are based on relative performance.

Panel B reports the primary reasons scientists dislike the changes in their tasks. The most common complaint is skill underutilization (73%), followed by tasks becoming less creative and more repetitive (53%). Concerns over credit allocation and the complexity of the AI tool were cited by 21% and 19% of researchers, respectively. These findings highlight the challenge of adapting to rapid technological progress. As one scientist noted: "While I was impressed by the performance of the [AI tool]...I couldn't help feeling that much of my education is now worthless. This is not what I was trained to do."

### 7.2 Beliefs About Artificial Intelligence

In addition to affecting job satisfaction, working with the model changes scientists' beliefs about artificial intelligence. Figure 13 shows researchers' level of agreement with five AI-related statements before and after the tool's introduction, revealing shifts along several dimensions. As discussed in Section 3, the survey was conducted after scientists had gained access to the model. Therefore, all pre-treatment beliefs represent respondents' best recollection.

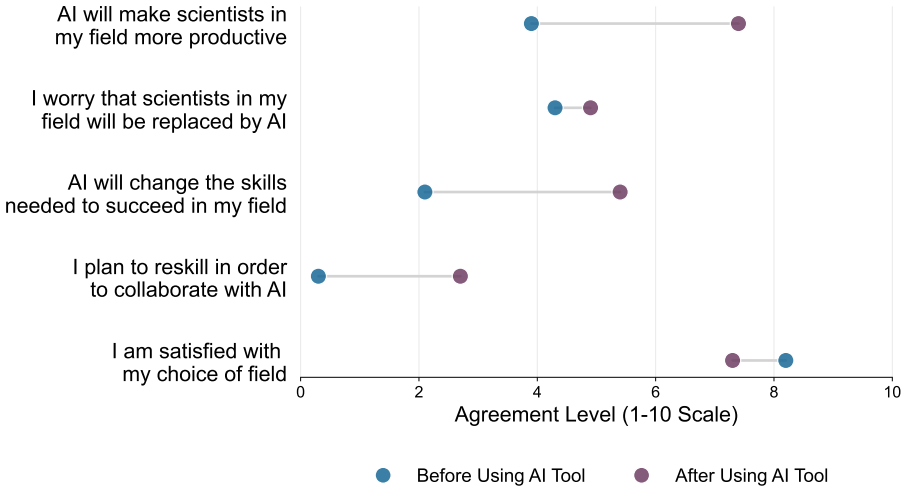



**Figure 13.** Shifts in Scientists' Beliefs About AI

*Notes:* This figure reports the change in researchers' beliefs about AI before and after using the tool. It shows five statements related to AI's impact on science and scientists. Agreement levels are measured on a 1-10 scale, shown on the x-axis. Each statement is represented by a pair of dots: blue dots indicate beliefs before using the AI tool, while red dots represent beliefs after using it. The information was collected after the experiment was completed, so pre-AI beliefs are based on scientists' best recollection. The relevant survey questions are provided in Appendix C.

Researchers report a significant increase in their belief that AI will enhance productivity in their field. Interestingly, concern over AI displacing jobs remains relatively stable, possibly reflecting the

fact that the model creates new tasks. Due to the changing research process, scientists indicate a significant increase in their belief that AI will alter the skills needed to succeed. Consequently, the proportion of researchers planning to reskill grows substantially. Finally, scientists report a small reduction in satisfaction with their choice of field.

These results show that hands-on experience with AI can profoundly influence views on the technology. Furthermore, the responses reveal an important fact: scientists did not anticipate the effects documented in this paper. This fits a recurring pattern of domain experts underestimating the capabilities of AI in their respective fields (Grace et al., 2018; Bostock, 2022; Grace et al., 2022; Steinhardt, 2022; Cotra, 2023).

## 8 Conclusion

The long-run impact of artificial intelligence hinges on the extent to which AI technologies transform science and innovation. This paper takes the first step toward answering this question, studying the randomized introduction of a new materials discovery tool in a large R&D lab. I find that AI substantially boosts materials discovery, leading to a rise in patent filing and an increase in downstream product innovation. However, the technology is effective only when paired with sufficiently skilled scientists.

Investigating the mechanisms behind these results, I show that AI automates a majority of idea generation tasks, reallocating researchers to the new task of evaluating model-produced candidate compounds. Top scientists learn to prioritize promising AI suggestions, while others waste significant resources testing false positives. Interpreted through the lens of a task framework, this shows that AI changes the skills required to make scientific discoveries.

Consequently, my findings speak to a broader debate about human expertise and creativity in a world of artificial intelligence (Brynjolfsson and McAfee, 2014; Daugherty and Wilson, 2018; Acemoglu and Restrepo, 2019; Autor et al., 2023). One perspective—often associated with the AI research community—posits that the combination of big data and deep learning will render domain knowledge obsolete, as models automate the majority of cognitive labor (Anderson, 2008; Grace et al., 2022; Schulman, 2023; Aschenbrenner, 2024). In contrast, others are pessimistic about AI's potential to perform economically valuable tasks, particularly in areas such as scientific discovery that require creative leaps (Woodie, 2022; Acemoglu, 2024; Wolfram, 2024). My results suggest an intermediate view. In materials science, I show that AI can meaningfully accelerate invention. However, the model must be complemented by domain experts who can evaluate and refine its predictions.

My analysis leaves several key issues unexplored. First, it is important to investigate the equilibrium effects on the supply and demand for scientific expertise. Second, while I consider one organizational adaptation to AI—hiring and firing practices—I do not study changes in training or incentives. Finally, it is critical to understand how the results change as AI improves.

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# A Additional Tables and Figures

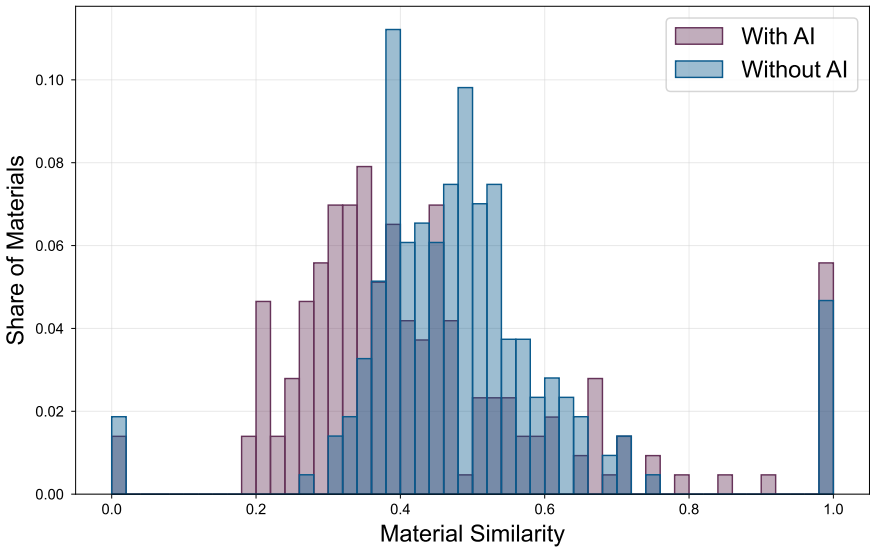



**Figure A1.** Distribution of Material Similarity

*Notes:* This figure shows the distribution of material similarity for compounds created before and after the introduction of AI. The similarity scores are calculated using the approach of De et al. (2016) described in Appendix B. These scores are only calculated for the crystals in my sample, which comprise 64% of all materials.

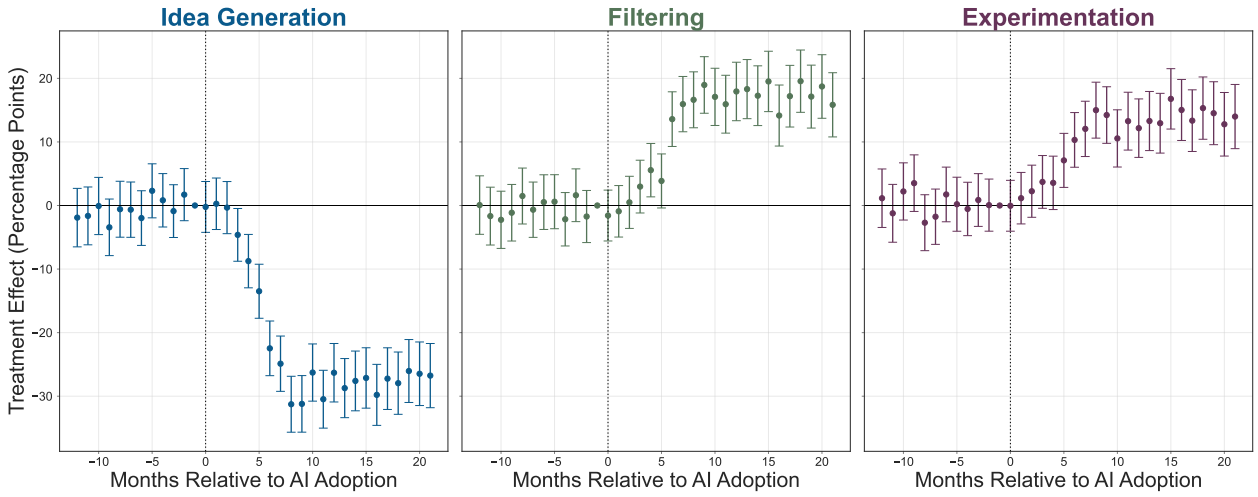



**Figure A2.** Impact of AI on the Composition of Research Tasks

*Notes:* This figure plots event studies for the impact of AI on the composition of research tasks. The estimates come from the following specification: $y_{it} = \alpha_i + \gamma_t + \sum_{k \in \mathcal{K}} \delta_k D_{i,t-k} + \beta' X_{it} + \varepsilon_{it}$ where I include a full set of fixed effects and controls. The outcomes are the percentage of scientist-hours spent on idea generation tasks, filtering tasks, and experimentation tasks, respectively. The process for classifying research tasks into these categories is discussed in Appendix B.5. I report 95% confidence intervals that are clustered at the team-by-month level.

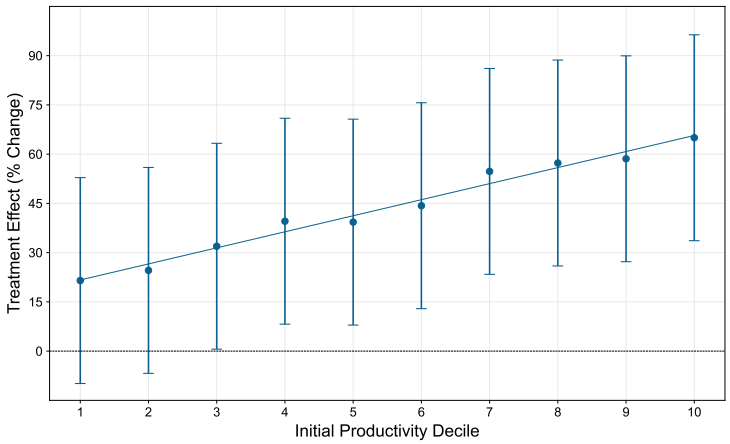



**Figure A3.** Team-Level Heterogeneity Estimates for Materials Discovery

*Notes:* This figure shows shows the heterogeneous impact of AI on materials discovery at the team. I use an equivalent specification as the one described in Section 5, interacting AI access with quantile dummies of initial productivity. However, all variables are now aggregated to the team-level. I report 95% confidence intervals based on standard errors clustered at the team level.

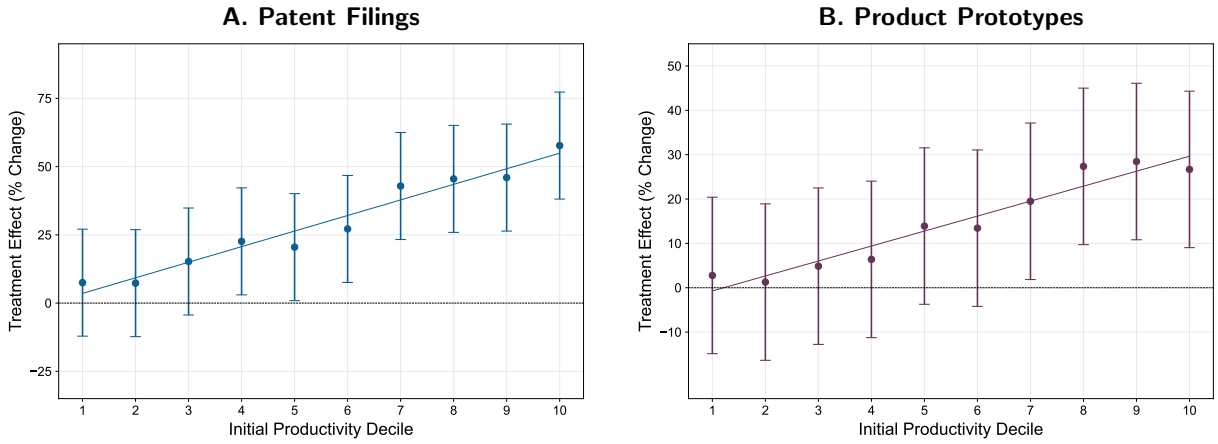



**Figure A4.** Heterogeneous Impact on Downstream Outcomes

*Notes:* This figure shows shows the heterogeneous impact of AI on downsteam outcomes across the scientist productivity distribution. Panel A shows estimates for patent filings and Panel B shows estimates for product prototypes. I use an identical specification as the one described in Section 5, interacting AI access with quantile dummies of initial productivity. The vertical lines represent 95% confidence intervals based on standard errors clustered at the scientist level.

| | Materials Discovery (1) | Materials Discovery (2) | Materials Discovery (3) | Materials Discovery (4) |
|---|---|---|---|---|
| Access to AI | 0.195*** | 0.212*** | 0.204*** | 0.208*** |
| | (0.105) | (0.092) | (0.078) | (0.065) |
| Team Fixed Effects | | ✓ | ✓ | ✓ |
| Month Fixed Effects | | ✓ | ✓ | ✓ |
| Time-Varying Team Characteristics | | | ✓ | ✓ |
| Material Type Fixed Effects | | | | ✓ |
| Intended Application Fixed Effects | | | | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 | 221 |

**Table A1.** Average Treatment Effect Under Alternative Specifications: Materials Discovery

*Notes:* This table reports average treatment effect estimates on materials discovery under different model specifications. Standard errors in parentheses are clustered at the team level. Column (1) includes no controls. Column (2) adds team and month fixed effects. Column (3) further includes controls for time-varying team characteristics. Column (4) adds fixed effects for material type and intended application. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

| | Patent Filings (1) | Patent Filings (2) | Patent Filings (3) | Patent Filings (4) |
|---|---|---|---|---|
| Access to AI | 0.049*** | 0.051*** | 0.048*** | 0.050*** |
| | (0.018) | (0.016) | (0.014) | (0.012) |
| Team Fixed Effects | | ✓ | ✓ | ✓ |
| Month Fixed Effects | | ✓ | ✓ | ✓ |
| Time-Varying Team Characteristics | | | ✓ | ✓ |
| Patent Category Fixed Effects | | | | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 | 221 |

**Table A2.** Average Treatment Effect Under Alternative Specifications: Patent Filings

This table reports average treatment effect estimates on patent filings under different model specifications. Standard errors in parentheses are clustered at the team level. Column (1) includes no controls. Column (2) adds team and month fixed effects. Column (3) further includes controls for time-varying team characteristics. Column (4) adds fixed effects for patent type and technology field. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

| | Product Prototypes (1) | Product Prototypes (2) | Product Prototypes (3) | Product Prototypes (4) |
|---|---|---|---|---|
| Access to AI | 0.024** | 0.026** | 0.023** | 0.025** |
| | (0.015) | (0.014) | (0.013) | (0.012) |
| Team Fixed Effects | | ✓ | ✓ | ✓ |
| Month Fixed Effects | | ✓ | ✓ | ✓ |
| Time-Varying Team Characteristics | | | ✓ | ✓ |
| Product Category Fixed Effects | | | | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 | 221 |

**Table A3.** Average Treatment Effect Under Alternative Specifications: Product Prototypes

This table reports average treatment effect estimates on product prototypes under different model specifications. Standard errors in parentheses are clustered at the team level. Column (1) includes no controls. Column (2) adds team and month fixed effects. Column (3) further includes controls for time-varying team characteristics. Column (4) adds fixed effects for product category. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

| | Materials Discovery (1) | Patent Filings (2) | Product Prototypes (3) |
|---|---|---|---|
| Access to AI | 0.231** | 0.055** | 0.025** |
| | (0.092) | (0.022) | (0.010) |
| Team Fixed Effects | ✓ | ✓ | ✓ |
| Month Fixed Effects | ✓ | ✓ | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 |

**Table A4.** Estimates Using Randomization Inference

*Notes:* This table shows average treatment effects with 95% confidence constructed using permuation tests, following Imbens and Rubin (2015). All regressions include team and month fixed effects. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

| | Point Estimate (1) | Standard Error (2) | Lower Confidence Bound (95%) (3) | Upper Confidence Bound (95%) (4) |
|---|---|---|---|---|
| *Panel A: Materials Discovery* | | | | |
| Borusyak et al. (2024) | 0.205 | 0.028 | 0.150 | 0.260 |
| Callaway and Sant'Anna (2021) | 0.212 | 0.025 | 0.163 | 0.261 |
| de Chaisemartin and D'Haultfœuille (2020) | 0.198 | 0.021 | 0.157 | 0.239 |
| Sun and Abraham (2021) | 0.208 | 0.027 | 0.155 | 0.261 |
| *Panel B: Patent Filings* | | | | |
| Borusyak et al. (2024) | 0.052 | 0.018 | 0.017 | 0.087 |
| Callaway and Sant'Anna (2021) | 0.054 | 0.015 | 0.025 | 0.083 |
| de Chaisemartin and D'Haultfœuille (2020) | 0.048 | 0.011 | 0.026 | 0.070 |
| Sun and Abraham (2021) | 0.051 | 0.017 | 0.018 | 0.084 |
| *Panel C: Product Prototypes* | | | | |
| Borusyak et al. (2024) | 0.026 | 0.008 | 0.010 | 0.042 |
| Callaway and Sant'Anna (2021) | 0.028 | 0.005 | 0.018 | 0.038 |
| de Chaisemartin and D'Haultfœuille (2020) | 0.022 | 0.001 | 0.020 | 0.024 |
| Sun and Abraham (2021) | 0.027 | 0.007 | 0.013 | 0.041 |

**Table A5.** Robustness to Alternative Estimators

*Notes:* This table shows the impact of AI on materials discovery (Panel A), patent filings (Panel B), and product prototypes (Panel C) using robust difference-in-differences estimators proposed by Borusyak et al. (2024), Callaway and Sant'Anna (2021), de Chaisemartin and D'Haultfœuille (2020), and Sun and Abraham (2021). All regressions include team and month fixed effects. Standard errors are clustered at the team level.

| | Materials Discovery | Patent Filings | Product Prototypes |
|---|---|---|---|
| | (1) | (2) | (3) |
| Access to AI | 0.225** | 0.062** | 0.029** |
| | (0.098) | (0.025) | (0.012) |
| Team Fixed Effects | ✓ | ✓ | ✓ |
| Month Fixed Effects | ✓ | ✓ | ✓ |
| Number of Scientists | 1,018 | 1,018 | 1,018 |
| Number of Teams | 221 | 221 | 221 |

**Table A6.** Estimates Excluding Untreated Teams Working on Same Material-Application

*Notes:* This table shows average treatment effects with 95% confidence intervals constructed using permutation tests, following Imbens and Rubin (2015). All regressions include team and month fixed effects. *, **, and *** indicate significance at the 10%, 5%, and 1% levels.

# B Data Appendix

## B.1 Data Sources and Definitions

I supplement the lab's internal data with several publically available datasets.

#### Materials Databases

## B.2 Measuring Material Quality

I measure the quality of materials based on their properties. Scientists begin the search process by defining a set of target features for each compound. These features vary signifiantly across materials, but often include both atomic and large-scale characteristics determined by the intended application. For example, researchers may target the band gap (the energy difference between the valence band and the conduction band) or the refractive index (how much a material bends light). For each feature, I calculate the absolute distance between the target and its realized value. I combine these distances into two indices capturing quality at the atomic and macro scales, as well as an overall index.

Concretely, given a material $m$ with $K$ target features, I follow the chemical informatics literature and define the quality index as:

$$Q_m = \left( \frac{1}{K} \sum_{k=1}^{K} \frac{\left( p_{k,m} - t_k \right)^2}{\sqrt{\frac{1}{M-2} \sum_{m' \neq m} \left( p_{k,m'} - \bar{p}_{k,-m} \right)^2}} \right)^{-1}$$

where $p_{1,m}, \ldots, p_{k,m}$ are the relevant properties of material $m$ and $t_1, \ldots, t_k$ are the targets.[16] The distance metric is rescaled by the leave-out standard deviation of each property across all materials tested, allowing aggregation across different types of features. Additionally, the index is normalized by the number of characteristics to support comparisons across materials with different numbers of target features. Across materials, the average number of target features is 4.7.

## B.3 Measuring Structural Similarity

The similarity between crystal structures is calculated in four steps:

1. Define the substructure of crystal $i$ to be the minimal repeating configuration of atoms and

[16] For features with unbounded targets, I set $t_k \in \{-\infty, \infty\}$.

bonds, denoted $s_j$. Let $\mathcal{A}_i$ be the set of atoms in the substructure. Let $d_i(a_i)$ be the physical distance of atom $a_i \in \mathcal{A}_i$ from the centroid of $s_i$.

2. For two atoms $a_i$ and $a_j$, define their chemical replaceability as $r(a_i, a_j) \in [0, 1]$. This is a scalar capturing the change in material properties when atom $a_i$ is replaced with atom $a_j$. The substitutability of two identical atoms is 1, and it decreases to a minimum of 0. Following De et al. (2016), the values of $r$ are taken from the experimental literature.

3. Given substructures $s_i$ and $s_j$, define a matching between the atoms in each substructure as a one-to-one function $m : \mathcal{A}_i \to \mathcal{A}_j$. If the substructures have different numbers of atoms, the surplus atoms in one set will be unmatched.

4. The similarity score for substructures $s_i$ and $s_j$ is defined as:

$$\text{Score}(s_i, s_j) = \max_m \sum_{\substack{a_i \in \mathcal{A}_i, a_j \in \mathcal{A}_j \\ \text{s.t. } a_j = m(a_i)}} r(a_i, a_j)^{\omega_r} \min\left(d_i(a_i), d_j(a_j)\right)^{\omega_c} \left\| d_i(a_i) - d_j(a_j) \right\|_2^{\omega_d}$$

   The sum is maximized over all possible matching of atoms in $s_i$ and $s_j$. The first term captures the chemical similarity of atoms $a_i$ and $a_j$. The second term puts additional weight on atoms that are closer to the centroid, reflecting the fact that central atoms are more predictive of material properties. The third term is the squared difference in the physical distance of $a_i$ and $a_j$ from their respective centroids, capturing geometric similarity between the structures. The weights $\omega_r$, $\omega_d$, and $\omega_d$ capture the relative importance of chemical similarity, centrality, and geomteric structure, respectively.[17]

5. Finally, the similarity measure is normalized to ensure that the metric is independent of the number of atoms in a substructure and has a scale between 0 and 1:

$$\text{Similarity}(s_i, s_j) = \text{Sigmoid}\left(\frac{\text{Score}(s_i, s_j)}{\sqrt{\text{Score}(s_i, s_i)\text{Score}(s_j, s_j)}}\right)$$

Figure A5 illustrates the approach. The image on the right shows the composition of a Zintl compound, a type of thermoelectric generator used in a range of electronics. Due to its crystalline structure, the material can be decomposed into substructures containing a central calcium ion surrounded by four aluminum antimonides. This set of atoms, combined with the distance of each peripheral ion from the central node, represents the information used in the similarity score.

[17] Following De et al. (2016), I set $\omega_r = .6$, $\omega_d = .13$, and $\omega_d = .27$. However, the novelty results are robust to the choice of weights.

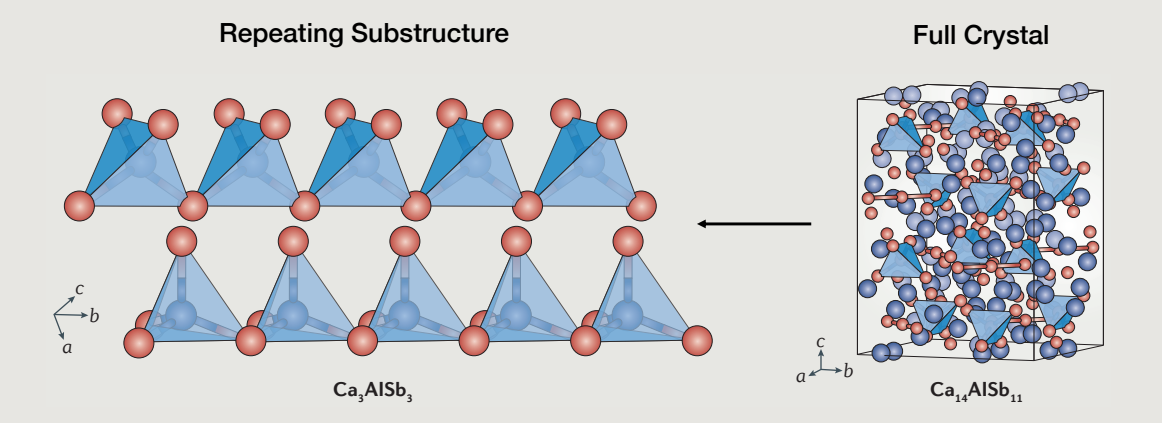



**Figure A5.** Example of a Crystal Material and its Substructure

Following this method, I calculate the similarity between newly discovered compounds and existing materials. The structure of known materials comes from the Materials Project (Jain et al., 2013), which maintains a database of more than 150,000 unique crystals.[18] Figure A1 shows the distribution of similarity for new crystals in my sample. The measure displays a somewhat trimodal distribution: the majority of materials follow a right skewed distribution centered around 0.45, while the rest are concentrated in a large mass near 1 and smaller peak near 0.

This method constructs a measure of similarity between atomic environments using Smooth Overlap of Atomic Positions (SOAP) kernels. The approach is designed to compare the local arrangements of atoms in materials or molecules, providing a way to quantify how similar different atomic environments are to each other.

The process begins by representing the local density of atoms around a central point. This density is described as a sum of Gaussian functions centered on each atom:

$$\rho_{\mathcal{X}}(\mathbf{r}) = \sum_{i \in \mathcal{X}} \exp\left(-\frac{(\mathbf{x}_i - \mathbf{r})^2}{2\sigma^2}\right) \tag{A1}$$

Here, $\mathcal{X}$ represents an atomic environment, $\mathbf{x}_i$ are the positions of atoms in this environment, and $\sigma$ is the width of the Gaussian functions. This representation smooths out the discrete atomic positions into a continuous density field.

The SOAP kernel, which measures the similarity between two environments $\mathcal{X}$ and $\mathcal{X}'$, is defined as:

$$\tilde{k}(\mathcal{X}, \mathcal{X}') = \int d\hat{R} \left[\int \rho_{\mathcal{X}}(\mathbf{r}) \rho_{\mathcal{X}'}(\hat{R}\mathbf{r}) d\mathbf{r}\right]^n \tag{A2}$$

[18]The Materials Project database is publically available at https://next-gen.materialsproject.org/.

This integral compares the overlap of the density fields for all possible rotations $\hat{R}$ of one environment relative to the other. The exponent $n$ (typically set to 2) helps to amplify the sensitivity to structural differences.

To ensure that the self-similarity of any environment is unity, the kernel is normalized:

$$k(\mathcal{X}, \mathcal{X}') = \frac{\tilde{k}(\mathcal{X}, \mathcal{X}')}{\sqrt{\tilde{k}(\mathcal{X}, \mathcal{X})\tilde{k}(\mathcal{X}', \mathcal{X}')}} \tag{A3}$$

To make the computation of this kernel tractable, the atomic density is expanded in terms of spherical harmonics and radial basis functions:

$$\rho_{\mathcal{X}}(\mathbf{r}) = \sum_{bl\,m} c_{bl\,m} g_b(|\,\mathbf{r}\,|) Y_{l\,m}(\hat{\mathbf{r}}) \tag{A4}$$

This expansion allows for the computation of a rotationally invariant "power spectrum":

$$p(\mathcal{X})_{b_1 b_2 l} = \pi \sqrt{\frac{8}{2l+1}} \sum_m (c^*_{b_1 l\,m}) c_{b_2 l\,m} \tag{A5}$$

The power spectrum encodes the structural information of the environment in a way that doesn't depend on its orientation.

Remarkably, the SOAP kernel can be expressed as a simple dot product of these power spectrum vectors:

$$k(\mathcal{X}, \mathcal{X}') = \hat{\mathbf{p}}(\mathcal{X}) \cdot \hat{\mathbf{p}}(\mathcal{X}') \tag{A6}$$

where $\hat{\mathbf{p}}$ represents the normalized power spectrum.

Finally, a distance between environments can be defined:

$$d(\mathcal{X}, \mathcal{X}') = \sqrt{2 - 2\hat{\mathbf{p}}(\mathcal{X}) \cdot \hat{\mathbf{p}}(\mathcal{X}')} \tag{A7}$$

This distance measure quantifies how different two atomic environments are. It has the properties of a proper metric, meaning it can be used to rigorously compare and classify atomic structures in materials science applications.

### B.4 Measuring Patent Novelty

I employ two patent similarity measures, proposed by Kelly et al. (2021) and Kalyani (2024).

### B.4.1 Kelly et al. (2021) Measure

Kelly et al. (2021) construct a measure of patent similarity based on the full text of patents. It follows a modified term frequency-inverse document frequency (TF-IDF) approach. For a given patent $p$ and term $w$, the term frequency is defined as:

$$\text{TF}_{pw} = \frac{c_{pw}}{\sum_k c_{pk}}$$

where $c_{pw}$ is the count of term $w$ in patent $p$. To account for the temporal nature of patent filings, it employs backward inverse document frequency (BIDF) for term $w$ in year $t$:

$$\text{BIDF}_{wt} = \log\left(\frac{\#\text{ patents prior to } t}{1 + \#\text{ documents prior to } t \text{ that include term } w}\right)$$

The modified TF-BIDF for patent $i$ and term $w$ is then defined as:

$$\text{TFBIDF}_{w,i,t} = \text{TF}_{w,i} \times \text{BIDF}_{w,t}$$

where $t = \min(\text{filing year for } i, \text{filing year for } j)$ when comparing patents $i$ and $j$. The TFBIDF vectors are normalized to unit length:

$$V_{i,t} = \frac{\text{TFBIDF}_{i,t}}{||\text{TFBIDF}_{i,t}||}$$

Finally, the similarity between patents $i$ and $j$ is computed as the cosine similarity of their normalized vectors:

$$\rho_{i,j} = V_{i,t} \cdot V_{j,t}$$

This measure $\rho_{i,j}$ lies in the interval $[0, 1]$, with higher values indicating greater similarity.

### B.4.2 Kalyani (2024) Measure

Kalyani (2024) constructs a measure of patent creativity based on the share of previously unused technical terms. The process involves two main steps: identifying technical bigrams and measuring whether they appear in existing patents.

Each patent is decomposed into bigrams, considering only those that appear at least twice in a patent and do not contain filler words. Technical bigrams are identified by removing non-technical bigrams (derived from the Corpus of Historical American English pre-1900) from each patent's

bigram list. For a patent $p$ filed in year $t$, a bigram $b$ is classified as creative at time $t$ if:

$$\text{Creative bigram}_{b,t} = \vec{1}\{b \notin \mathbb{B}'_{t-5,\ldots,t-1}\}$$

where $B'_{t-5,\ldots,t-1}$ is the set of bigrams appearing in patents filed in the previous five years. Patent creativity is then calculated as:

$$\text{PatentCreativity}_p = \frac{1}{|B_p|} \sum_{b=1}^{B_p} \vec{1}\{b \notin \mathbb{B}'_{t-5,\ldots,t-1}\}$$

where $B_p$ is the set of bigrams in patent $p$. The measure is standardized by the average in a technology class throughout the sample.

## B.5 Classifying Research Tasks

This section details the procedure for classifying textual data on scientist activities into categories of research tasks.

### B.5.1 Scientist Activities Data

Scientists record their activities in logs required for administrative purposes. Each entry contains three components: entry date, duration of activity, and textual description. On average, scientists record 5.8 entries per week. Across scientists, this amounts to more than 11 million entries over my entire sample.

To transform this textual information into a meaningful quantitative metric, I separate the materials discovery process into three categories of tasks: idea generation, filtering, and experimentation. Idea generation encompasses activities related to developing potential compounds, such as reviewing the literature on existing materials or creating preliminary designs. Filtering tasks focus on selecting which compounds to advance, often involving the analysis of simulations or predicting material characteristics based on domain knowledge. Finally, experimentation tasks are dedicated to synthesizing new materials and conducting tests to evaluate their properties. Based on the materials science literature and discussions with the lab's scientists, these categories divide the discovery process into meaningful, high-level groups.

### B.5.2 Classification with Large Language Model

I employ a large language model—Claude 3.5 Sonnet—to classify the textual descriptions of research activities. Compared to other frontier models, such as GPT-4, GPT-4o, or Claude 3 Opus,

Claude 3.5 displays considerably better performance. The prompt is structured as follows:

**Prompt:** You are a materials science research activity classifer AI. Analyze the given materials discovery research activity and output in JSON format with keys:

- classification: (Idea Generation/Filtering/Experimentation/Other)
- certainty: (integer from 1 to 10, where 1 is least certain and 10 is most certain)

Research activity to classify: [Research Activity Description]
Analyze the activity in the context of materials science and materials discovery, then provide your classification and certainty level in the specified JSON format. Always choose one of the four categories for the classification, even if you're uncertain.

**Claude 3.5 Sonnet:**

```
{
  "classification": "[Category]",
  "certainty": [1-10]
}
```

The prompt includes several features that improve the LLM's accuracy. First, I ask for the response in JSON format to ensure standardization.

### B.5.3 Validation

| Category | True Positive Rate | False Positive Rate | True Negative Rate | False Negative Rate |
|---|---|---|---|---|
| Idea Generation | 21.3 | 3.8 | 70.2 | 4.7 |
| Filtering | 17.6 | 2.4 | 74.3 | 5.7 |
| Experimentation | 18.9 | 4.9 | 71.4 | 4.8 |
| Other | 15.1 | 6.2 | 72.8 | 5.9 |

**Table A7.** Research Task Classification Accuracy

#### B.5.4 Measuring New Research Tasks

# C Survey Details

## C.1 Survey Questions

### C.1.1 Introduction

Welcome and thank you for participating! We appreciate your willingness to share your experience with the newly implemented AI tool in your lab. This 15-minute survey aims to gather feedback on how the tool has been integrated into the materials discovery processes and how it has impacted your work.

Your accurate responses will play an important role in our lab's future decisions about AI use, such as changes to training and management practices. Please note that all responses to this survey are anonymous. We value your honest feedback as it is essential to improve our scientists' experience with the AI tool.

### C.1.2 Background Questions

1. We will start by asking you a few questions about your background and role in the lab. Which of the following, if any, best describes your role in the lab?

    - Research Scientist
    - Lab Technician
    - Administrator
    - Other (please specify)

2. Is your research primarily focused on discovering or synthesizing new materials?

    - Yes
    - No

3. We will now ask a few questions about your use of the AI tool. Throughout the survey, "AI tool" refers to the new deep learning model recently introduced in your lab.

    Please indicate the date when you first gained access to the AI tool.

4. Please indicate the date when you first started using the AI tool in your work.

### C.1.3 Questions About Use of AI Tool

5. Think about your current process for discovering materials. How important is the AI tool in this process?

    - Not at all important
    - Slightly important
    - Moderately important
    - Very important
    - Extremely important

6. Based on your experience working with the AI tool, indicate your level of agreement with the following statements:

    - The complexity of the AI tool makes it difficult to understand.
    - The complexity of the AI tool makes it hard to trust its results.
    - Compared to other methods I have used, the AI tool generates potential materials that are more likely to possess desirable properties.
    - The AI tool generates potential materials with physical structures that are more distinct than those produced by other methods I have used.

    (Scale: Strongly disagree, Somewhat disagree, Neither agree nor disagree, Somewhat agree, Strongly agree)

7. Consider the tasks you typically perform in your job. Think about the percentage of your work hours dedicated to the following categories:

    - *Generating ideas for potential materials:* This category includes activities like reviewing literature on existing materials or creating preliminary designs.
    - *Deciding which potential materials to test:* This category includes activities like analyzing simulation results or predicting which materials will be easy to synthesize.
    - *Synthesizing materials and testing their properties:* This category includes activities like preparing compounds or conducting experiments to test material properties.
    - *Other:* This category include any tasks involved in the process of discovering materials that do not fall into the previous categories.

Answer the following questions as accurately as you can, based on your best recollection.

In the last three months, what percentage of your work hours were dedicated to the following categories?

- Generating ideas for potential materials
- Deciding which potential materials to test
- Synthesizing materials and testing their properties
- Other

8. Before the introduction of the AI tool, what percentage of your work hours were dedicated to the following categories?

    - Generating ideas for potential materials
    - Deciding which potential materials to test
    - Synthesizing materials and testing their properties
    - Other

9. On a scale of 1 to 10, how effective are you in each category of task?

    - Generating ideas for potential materials
    - Deciding which potential materials to test
    - Synthesizing materials and testing their properties

10. On a scale of 1 to 10, how effective are you in each category of task relative to other members of your team? (Same categories as above)

11. Think about how you select which AI-generated material candidates to synthesize and test. Answer the following questions based on your experience working with the AI tool.

    Compared to previous methods, how would you rate the difficulty of evaluating AI-generated candidate materials?

    - Much easier
    - Somewhat easier
    - About the same
    - Somewhat harder
    - Much harder

12. How frequently can you identify an AI-suggested candidate compound as a false positive without attempting to synthesize the material?

    - Never
    - Rarely
    - Sometimes
    - Often

13. On a scale of 1 to 10, how useful are each of the following for evaluating AI-generated candidate materials?

    - Past scientific training
    - Past experience with similar materials
    - Intuition or gut feeling
    - Experience with similar AI tools

14. Please provide any additional comments you would like to share on your experience selecting AI-generated candidate materials for testing. (Text entry)

#### C.1.4 Questions About Job Satisfaction

15. Next, we will ask a few questions about how you enjoyed working with the AI tool.

    Compared to your previous workflow, how enjoyable is your work after gaining access to the AI tool on a scale of 1 to 10?

16. Think about the impact of the AI tool on your productivity. On a scale of 1 to 10, how enjoyable is your work as a result of this shift in productivity?

17. Think about the impact of the AI tool on the tasks you perform. On a scale of 1 to 10, how enjoyable is your work as a result of this shift in tasks?

18. What are the primary reasons that the AI tools makes your tasks less enjoyable? Please select all that apply.

    - My tasks are more repetitive
    - My tasks are less creative
    - My tasks underutilize my skills

- I experience technical issues using the AI tool
- I don't understand the AI tool
- The AI tool makes it harder to assign credit for discoveries
- Other (please specify)

19. Based on your best understanding, are promotion and compensation decisions in your lab primarily based on:

    - Absolute performance
    - Performance relative to other scientists
    - Other
    - Not sure

20. Please provide any additional comments you would like to share on how you enjoyed working with the AI tool and why. (Text entry)

#### C.1.5 Questions About Views on Artificial Intelligence

21. Finally, we will ask a few questions about how working with the AI tool has changed your views on artificial intelligence.

    Please report your current level of agreement with the following statements on a scale of 1 to 10:

    - AI will make scientists in my field more productive
    - I worry that scientists in my field will be replaced by AI
    - AI will change the skills needed to succeed in my field
    - I plan to reskill in order to collaborate with AI
    - I am satisfied with my choice of field

22. Based on your best recollection, please report your level of agreement with the following statements before using the AI tool on a scale of 1 to 10:

    - AI will make scientists in my field more productive
    - I worry that scientists in my field will be replaced by AI
    - AI will change the skills needed to succeed in my field
    - I plan to reskill in order to collaborate with AI

- I am satisfied with my choice of field

23. Please provide any additional comments on how working with the AI tool has changed your views. (Text entry)

## C.2 Respondent Characteristics and Attrition

**Table A8.** Characteristics of Survey Sample

| | Respondents | Non-Respondents |
|---|---|---|
| ***Scientist Characteristics*** | | |
| Age (Years) | 42.87 | 46.12 |
| Tenure at Firm (Years) | 8.33 | 10.58 |
| ***Education*** | | |
| Share Bachelors Degree | 0.04 | 0.07 |
| Share Masters Degree | 0.32 | 0.34 |
| Share Doctoral Degree | 0.64 | 0.59 |
| ***Education Field*** | | |
| Share Chemical Engineers | 0.24 | 0.20 |
| Share Chemists | 0.15 | 0.13 |
| Share Materials Scientists | 0.22 | 0.24 |
| Share Other Fields | 0.27 | 0.34 |
| Share Physicists | 0.12 | 0.09 |
| ***Material Type*** | | |
| Share Biomaterials | 0.25 | 0.25 |
| Share Ceramics and Glasses | 0.19 | 0.19 |
| Share Metals and Alloys | 0.31 | 0.32 |
| Share Polymers | 0.24 | 0.24 |
| ***Innovative Output*** | | |
| New Materials (Yearly) | 0.79 | 0.89 |
| Patent Filings (Yearly) | 0.20 | 0.24 |
| Product Prototypes (Yearly) | 0.27 | 0.32 |
| ***Sample Size*** | | |
| Number of Scientists | 447 | 571 |

| Question Number | Number of Responses |
|---|---|
| Question 1 (Required) | 447 |
| Question 2 (Required) | 447 |
| Question 3 (Required) | 447 |
| Question 4 (Required) | 447 |
| Question 5 | 445 |
| Question 6 | 445 |
| Question 7 | 442 |
| Question 8 | 440 |
| Question 9 | 440 |
| Question 10 | 438 |
| Question 11 | 435 |
| Question 12 | 435 |
| Question 13 | 432 |
| Question 14 | 428 |
| Question 15 | 425 |
| Question 16 | 425 |
| Question 17 | 420 |
| Question 18 | 415 |
| Question 19 | 415 |
| Question 20 | 408 |
| Question 21 | 402 |
| Question 22 | 395 |
| Question 23 | 388 |

**Table A9.** Responses per Survey Question

# D Model Derivations

## D.1 Optimal Task Allocation

## D.2 Proof of Proposition 1

## D.3 Proof of Proposition 2

## D.4 Proof of Proposition 2

## D.5 Proof of Proposition 4