

Epistemic Gaps and the Attribution of (AI) Discovery

Eamon Duede^{△*1, 2} and Daniel C. Friedman^{△†1}

¹Purdue University

²Argonne National Laboratory

Abstract

What does it take to properly recognize someone as having made a scientific discovery? According to the *Cognitivist*, discovery attribution properly depends on the exercise of distinctive cognitive capacities such as competence, meta-reflective awareness, or domain-general understanding. Since AI systems lack such capacities, they cannot, on this view, be discoverers. If the Cognitivist is right, AI-driven science will be a markedly impoverished enterprise. Here, we argue otherwise. We develop an alternative, non-cognitivist conception of scientific discovery according to which discovery turns on successfully negotiating epistemic gaps. This reconception, we argue, better captures both familiar human cases and novel AI contributions, thereby re-framing the grounds for attributions of discovery in contemporary science. AI systems, we argue, can be appropriately attributed scientific discoveries. Along the way we develop a general moral for philosophical reflection in the age of AI-infused science.

1 Introduction

Despite prominent and successful deployments in mathematics [DVB⁺21, RPBN⁺24, TWL⁺24], structural biology [JEP⁺21a], quantum chemistry [GBAIH⁺16], materials science [TDW⁺19], sociology [KTE19], and many other areas of research, scientists and philosophers agree that, in general, artificial intelligence systems (AIs) for science are, in important respects, still quite limited. Such agreement is important, but attending to

*Email: eduede@purdue.edu

†Email: dcfriedm@purdue.edu

[△]These authors contributed equally to this work.

issues about which philosophers and scientists *disagree* is often more instructive. One such issue concerns whether AIs are, themselves, capable of making genuine scientific discoveries. This issue forces reflection not just on specific capacities of AIs, but the nature of scientific discovery.

Scientists are generally quite comfortable ascribing scientific breakthroughs to AIs. Some have even gone so far as to suggest that AIs be considered for scientific honors and prizes [Wan25]. Philosophers, however, are more reserved. Typically, philosophers argue that AIs lack the core capacities necessary for genuine scientific discovery. Which capacities are these? The list is long, diverse, and conspicuously *cognitive*. AI systems are said to lack sufficient disciplinary competence, meta-reflective and imaginative capacities, as well as generalizable domain knowledge (e.g., world models) [Hal21, BG25, Stu19], some combination of which is taken to be required for *genuine* discovery. Without the capacities necessary for discovery, then, AI-driven science will be a markedly poorer enterprise, the “self-driving laboratory” of the future a decidedly impoverished place [Cra20].

The issue here runs deeper than just which systems (human or otherwise) to credit as discoverers. To see this, imagine critics are correct, AI systems cannot make discoveries. Nevertheless, we may well observe AI-driven science making important progress. We would then be forced to amend the pride of place discovery enjoys in our understanding of scientific progress. Discovery is often taken as the ideal outcome of a scientific episode, the success case for scientific inquiry [Sch25]. If science proceeds in leaps and bounds, but without discoveries, this requires radical and counterintuitive revision to core tenets in the philosophy of science.[△]

In this paper, we offer a defense of the possibility of AI scientific discovery, and in so doing, defend the epistemic promise of AI-driven science. Our account allows us to widen the scope of discovery in principled fashion, without thereby jettisoning our commitment to its role in scientific progress and as paradigm product of successful science. Importantly, to recognize an episode of discovery as attributable to an AI is not to recognize an AI as performing the role of a *scientist* —it is not to claim that AIs could reasonably be awarded prizes.

We argue that the issue lies not with the capacities (or lack thereof) of AI systems, but rather with a widespread, if quotidian, conception of scientific discovery that, admittedly, emerges quite naturally from observation of and reflection upon the history of science. After all, which genuine scientific discoveries of the past were not the achievement of an agent in possession of much that AIs likely lack? Nevertheless,

[△]The centrality of discovery is embraced by theorists as diverse as [Pop34, 32], who notes the game of science itself is the game of scientific discovery; [Kuh97] who sees discovery as often standing as an exemplar or undergirding shifts in paradigm; and [Fey93] who equates discovery with progress, as well as most contemporary thinkers concerned with the aims of science.

attending to clear cases of scientific contribution arising without many of these missing capacities demonstrates their contingency.

Our diagnosis: the purportedly necessary but missing capacities for discovery are, in fact, reflections of central features of *human* scientific discovery, not scientific discovery as such. As a description of a scientific enterprise shaped and undertaken by human scientists, such conflation is natural but misleading. Meaningful scientific discovery is likely well within reach of AI systems, not because they, in fact, have (or will soon have) capacities that they apparently lack. But, rather, because such capacities are simply non-essential.

Instead, discovery involves successful navigation of epistemic gaps. *Gap revealing* discoveries proceed by bringing anomalies or otherwise unexpected phenomena to light. *Gap bridging* discoveries proceed by moving from well specified problems to novel and previously untractable solutions.

Our conception of discovery as successful gap navigation deepens our understanding of *both* human and AI discoverers. Still, further reflection upon the quotidian conception of discovery is instructive. The function of the missing capacities is not entirely vestigial. They play important roles in the scientific eco-system.

Here's the plan: In §2, we consider three capacities purportedly necessary for an episode in the history of science to count as a scientific discovery. Because AIs lack these capacities, the thought goes, they cannot be recognized as scientific discoverers. Reflection on episodes of discovery involving humans offers reason to resist these arguments. In §3, we present clear episodes involving AIs making scientific contributions which we argue merit attributions of discovery. Comparison of these AI cases with human cases highlights a deeper pattern. This pattern renders visible that discovery consists in *successfully negotiating epistemic gaps*, either by revealing them (like X-rays, precession of Mercury, and Pulsars) or by spanning them (like *Tiktaalik*, protein folding, and online bin packing). Since AI systems make contributions which successfully negotiate these epistemic gaps, AIs can make scientific discoveries (§4). However, in §5, we explore a social condition for discovery that AI systems may fail to meet. In §6, we reflect on the important role these missing capacities may play if not as essential features of scientific discovery. We close by reflecting on the impact of our arguments for AI-driven science and philosophical understanding of scientific inquiry in §7.

2 Variations on a Cognitivist Theme

Terracotta Army: In early 1974, a group of farmers digging a well in Lintong County near Xi'an, Shaanxi province, struck fragments of clay while working their land. The fragments looked like broken bits of pottery and sculpted

body parts with no immediate use or explanation, belonging, perhaps, to patterned, life-sized human figures. Upon evaluation by archaeologists, the fragments were determined to be part of a vast subterranean funerary complex, the first of its kind to have been uncovered—a Terracotta Army, standing sentry before the tomb of China’s First Emperor, Qin Shi Huang [Led01].

Tiktaalik: In 2004, paleontologists Neil Shubin, Edward Daeschler, Farish Jenkins Jr., and their teams, after years of searching outcrops on Ellesmere Island in the Canadian Arctic, uncovered the fossilized remains of a long-sought transitional form between lobe-finned fish and early tetrapods. Careful excavation and analysis revealed a mosaic of features characteristic of the evolutionary shift from water to land. With fins and scales alongside a flat head, mobile neck, and robust rib bones, the specimen was determined to represent a new genus and species, the first of its kind to have been observed—*Tiktaalik*, entombed for an eon in Devonian strata [DSJJ06].

Pulsar: In late 1967, then second-year PhD student Jocelyn Bell Burnell noticed a regular irregularity in an input trend captured by the chart-recorder for a new radio telescope that she had been tasked with monitoring. The trend was irregular insofar as, in a single patch of sky, it recorded bursts that did not behave like the rest of the radio void. It was regular in that the bursts recurred with a fixed periodicity. Upon evaluation by Antony Hewish and others, it was determined that the source was a new kind of astrophysical object, the first of its kind to have been observed—a pulsar, PSR B1919+21 calling out faintly from Vulpecula in the northern sky [HBP⁺68].

Terracotta Army, *Tiktaalik*, and Pulsar each represent highly significant discoveries in the disciplines of archaeology, evolutionary biology, and astrophysics respectively. It is widely agreed that Daeschler, Shubin, and Jenkins discovered *Tiktaalik*, and, though she did not ultimately share the Nobel Prize with Hewish, Jocelyn Bell Burnell, indeed, discovered the Pulsar. Yet, on most accounts it seems natural and intuitive to say that the Lintong farmers did not, themselves, make a scientific discovery in finding the Terracotta Army.

Why do we naturally say that Daeschler, Shubin, Jenkins, and Bell Burnell made discoveries, while the Lintong farmers did not? The answer cannot lie simply in the importance of what was uncovered as both, say, PSR B1919+21 and the Terracotta Army fundamentally transformed their disciplines. Rather, to see Bell Burnell as a *discoverer* and the Lintong farmers as, say, mere finders has traditionally depended upon how we understand certain features of the *process* or *activity* that ultimately results in discovery.

Because discoveries are hard won, philosophical accounts have, quite reasonably, tended to focus on the cognitive *abilities* or *capacities* of discoverers. In fact, much mid-century philosophy of science took it as a given that, however it is that scientists arrive at discoveries, that process is best described or cashed out in psychological terms [Rei38, Pop14].

Recent work extends this line of argument to artificial intelligence. In addressing whether AIs can make discoveries, argument has centered on the role of the cognitive capacities of ‘competence’ (§2.1), ‘meta-reflection’ (§2.2), and ‘domain knowledge’ (§2.3). These capacities are taken to distinguish cases of genuine discovery like that of *Tiktaalik* from mere findings in cases like the Terracotta Army and, by analogy, from the contributions of contemporary AI systems. Call such approaches: *Cognitivist*.

A virtue of a Cognitivist approach is that it accords with intuitions about attributions of discovery in cases like the *Tiktaalik* and the Terracotta Army. Moreover, such an approach offers conceptual resources for classifying the contributions of AIs to episodes of science, concluding that, as of now, AIs are incapable of making scientific discoveries.

Despite their appeal, Cognitivist accounts face three serious shortcomings. First, they fail to reach the correct conclusion for a class of cases like Pulsar. Second, they lead to what we argue are bizarre conclusions regarding recent AI driven breakthroughs. Finally, they are at odds with scientific practice concerning AI contributions. To see this, we consider each of ‘competence’, ‘meta-reflection’, and ‘domain knowledge’ in turn. Doing so demonstrates how capacity focused accounts misfire, and lays the groundwork for an alternative view on which episodes of discovery are best understood as having resulted from the successful negotiation of epistemic gaps.

2.1 Competence

A natural way of distinguishing someone who has made a scientific discovery from someone who has merely stumbled upon something important is to see only the former as having exercised a kind of *competence* that is relevant to the outcome. On this view, genuine discoveries arise when a finding expresses the domain-relevant capacities of the discoverer, whereas mere findings are accidents, arrived at in a way unguided by disciplinary skill. Accordingly, Daeschler, Shubin, and Jenkins can be seen as having discovered *Tiktaalik* because their search expressed precisely the competences that evolutionary biology demands. By contrast, the Lintong farmers merely stumbled upon the Terracotta Army, their encounter completely unguided by any expression of archaeological competence.

As applied to AI in science, [BG25] argues that AI systems are incapable of making scientific discoveries because they lack sufficient competence for discovery. Specifically, [BG25, 4] defends the following competence principle:

Competence Principle: “For subject (or group) S’ finding F of object Y to count as a scientific discovery of Y, F should be linked to or express S’ competence concerning the field of discovery where Y belongs.”

More specifically, with respect to discovery, this principle is thought to be expressed in cases where either the finding is the result of recognizably domain-relevant reasoning or if the finder can, upon reflection, provide an explanation of the finding’s scientific relevance. Indeed, the *Competence Principle* captures why the Terracotta Army looks like a mere finding while *Tiktaalik* looks like a discovery. And, so, it seems that this principle picks out and reflects a general connection between the (domain-relative) scientific capacities exercised by a discoverer in making a finding, and that finding constituting a genuine discovery.

If one is committed to the idea that a capacity like that described by *Competence Principle* is required for discovery, then the question of whether anyone, including AIs, can be discoverers depends necessarily on whether they possess the relevant competencies. A principle of this kind would seem to rule out AIs insofar as any notion of *AI competence* is potentially misleading. AI outputs, the objection goes, are mere predictive efforts based on representation learning on a set of training data rather than deep knowledge of and possession of skills relevant to deploying the concept in question. Moreover, the way such training leads to output generation is notoriously opaque [Bog21, Cre20, Due23, Sul19]. Accordingly, because the process of training and subsequent process of output generation for many AI systems is something of a black-box, we have little way of knowing which features of the target phenomenon lead to the putative discovery. It may be the kinds of features whose picking out and salience we attribute to competence generating the output, or it may be other accidental or misleading features of the stimulus. So long as it is the latter, the output is not arrived at via, in an important sense, the AI system’s competence, and any resultant output cannot constitute a discovery.

Of course, reasoning in this way turns the question of whether AIs can be discoverers into an empirical issue. Commitment to something like *Competence Principle* can, at most, warrant suspension of judgment with respect to whether AIs express relevant competencies. If, so the thinking goes, we cannot determine positively that AI systems reason in such a way as manifests competence, we cannot attribute scientific discoveries to them. Moreover, AI systems are presently unable to offer meaningful explanations of the relevance of their outputs. Here too, the black-box nature of AI output generation impugns our understanding of the extent to which AI systems “grasp” why or how the output connects to a broader conceptual framework or theory. When an LLM, for instance, supplies reasons, there is no way of knowing that these are *its reasons*.

Of course, scientists are notorious for not knowing how they arrive at discoveries.[△] Their own reasoning is often opaque to *them* (and certainly to us). There are countless (probably apocryphal) stories like Kekulé’s discovery of the structure of benzene while dreaming of atoms dancing and forming chains in the midst of a foggy ouroboros.

But, more concretely, appeal to something like the *Competence Principle* fails to account for straightforward and well documented cases of discovery. Consider, again, Pulsar. When Bell Burnell first noticed the irregularity in the chart recorder, she was a second year PhD student, quite far from having acquired the kind of deep, disciplinary competence required for making sense of irregular recordings coming from a radio telescope. She thought what she was observing was “scruff”, could neither explain its significance, nor tell whether it was consistent or inconsistent with any specialized astrophysical model. What she could tell was that it was different from what she had been seeing coming off the recorder. Because Bell Burnell was inquisitive and motivated, she continued to investigate, brought her observations to the attention of Hewish, and came to understand *ex post* that she had made a discovery—its significance having been *explained to her*.

If exercise of a kind of competence demanded by *Competence Principle* is required to count as having made a scientific discovery, then, we should conclude that Bell Burnell did not discover the pulsar. Yet this is absurd. The subsequent controversy over the gender bias involved in failure to award Bell Burnell the Nobel Prize for this discovery (awarded instead to Hewish), shows that in a clear and intuitive sense, Bell Burnell discovered the pulsar [Wal]. Competence, we maintain, may quite often accompany discovery, but needn’t be thought essential to it. As a result, whether AIs count as scientific discoverers will not depend on whether they possess a competence capacity.

2.2 Meta-reflection

A discovery is an epistemic achievement. Plausibly then, for one’s finding to constitute a *genuine* epistemic achievement, it must involve awareness and appropriate sensitivity to one’s epistemic strengths and weaknesses [Sos]. In [BG25], this appears as a meta-reflection principle which, itself, depends on competence.[△] Such an appeal helps distinguish between *Tiktaalik* and Terracotta Army. The careful excavation and analysis proceeded the way they did because Shubin, Daeschler, and Jenkins Jr. were aware of the limitations (and power) of the tools at their disposal and used these tools and not others to predict where to search for the relevant fossils as well as how to identify

[△]This motivates, in part, the salience of the distinction between the context of discovery and the context of justification.

[△]In [BG25, 8], the Meta-Reflection Principle states that “For subject (or group) S’ finding F of object Y to count as a scientific discovery of Y, S should have reflective insights of their own competence in the field in which discoveries of Y are made.”

them. By contrast, the Lintong farmers deployed no reflective insight or awareness concerning their archaeological competence.

If a meta-reflective capacity is essential to count as a discoverer, this stands to rule out AI. AIs are not currently capable of (general) meta-reflection. Even computational approaches which implement something like meta-reflection will struggle to endow such systems with the capacity to evaluate how confident they should be in their output, nor to identify what data their training set would need to be supplemented with in order to make such evaluation possible (or unnecessary). Of course, AIs do output predictions ordered by probability. Still, very reasonable skepticism about the role of probability distribution estimates leads [BG25] to conclude that AIs fail to possess the relevant meta-reflective capacity, and thus cannot make discoveries.

Yet, in having already established that competence is not essential to discovery, it is not immediately clear what we might gain from claiming that meta-reflection is essential independent of competence. One thought is that, if some *specific* discovery depends on competence, then meta-reflection might be required to guide competence. But, absent competence, what purpose might meta-reflection serve? Presumably, the vast majority of historical cases of discovery involve highly competent scientists whose work, undoubtedly, reflects deep meta-reflective cogitation. But, not all.

When Bell Burnell first observed an irregularity in the chart-recorder's output, one can easily imagine that the only relevant reflective insight available to her was that she did not know what to think. The reading could be interference, a malfunction, her own error, significant, insignificant—on and on. Not knowing what exactly to think, she did what good scientists do and continued to gather data. Presumably, a sufficiently programmed AI, lacking any reflective capacity at all, might well do the same. Whatever meta-reflection amounts to, it cannot be an *essential* precondition of discovery.

2.3 Domain General Knowledge

It can seem nigh impossible to identify cases of scientific discovery involving discoverers who did not, in some way, possess deep knowledge of the relevant domain. In fact, the possession of domain-general knowledge has long been considered essential for application and expression of the capacity for problem-solving creativity [Dun97, NSS62, Sim04]. On this view, genuine discoveries arise not from narrow or task-specific expertise, but from the flexible application of a more general understanding to novel problem spaces. A discoverer must, as it were, be able to see the field from above in order to grasp how principles, methods, and heuristics might transfer across contexts. Moreover, scientists [Her24], social scientists [Cet99], and philosophers [Kuh97] alike have long maintained that domain general knowledge is required

in order to grasp which problems are worth pursuing, to spot anomalies, adhere to disciplinary norms of inquiry—on and on.

Such thinking motivates what we might call a *Domain Knowledge Principle*, which holds that for someone to count as having made a discovery in a particular domain, the discovery must have been, at least in part, the result of applying domain-general knowledge and understanding to the problem-space in which the discovery occurred. Such a principle straightforwardly makes sense of the difference between the discovery of *Tiktaalik* and the farmers' finding of the Terracotta Army. In the former case, the discoverers knew enough evolutionary biology, geology, and anatomy and physiology to know what was missing from the historical record, where it was likely to be found, and what phenotypic features it would possess. Nothing of the sort holds for the latter.

If a *Domain Knowledge Principle* is required for a finding to count as a discovery, the thought goes, we should suspend judgment about whether these AIs can count as discoverers. For instance, [Hal21] argues, even in cases of extremely impressive and creative AI problem solving, systems such as AlphaGO fail to possess the requisite domain-generality that is crucial in meaningful scientific insight. While AlphaGO might be exceptionally knowledgeable and creative within GO, it fails to translate such creativity and understanding to other relevant games. Interestingly, domain-generality is precisely what subsequent systems like AlphaZero excel at. But, perhaps, even more impressively, state of the art large language models all demonstrate and appear to instantiate, at a performance level, a kind of generality traditionally reserved for human cognition.

Given the creep of generality, commitment to something like the *Domain Knowledge Principle*, once again, transforms the question of whether AIs can count as discoverers from a general, philosophical question, into an empirical question about specific episodes involving AIs. If we understand such domain general knowledge as an important component of scientific discovery, then we should, from case to case, be skeptical AI systems can make scientific discoveries, insofar as their insight is often (but not always) domain limited and non-general.[△] But, such a shift to empirical considerations betrays the mistake—it relocates what is a conceptual question into a contingent question about machine capacities.

Similar skepticism should then equally apply to cases involving human scientists. Consider, once again Bell Burnell's discovery of PSR B1919+21. She did not identify the irregularity in the chart-recorder output as inconsistent with the epistemic commitments of astrophysics, nor did she exercise a capacity for creative problem-solving nurtured by exquisite sensitivity to the accumulated wisdom of her domain. Rather,

[△]While [Hal21] leaves open the precise relationship between creative problem-solving/insight and discovery, others in the literature such as [CK22], seem to treat the connection as at least one of necessity. We follow their lead.

she noticed that the “scruff” on the recorder was inconsistent with what she had observed from the rest of the, as it were, *radioscape*. This is not to deny that domain general knowledge is often, if not usually, central to discovery. It is, rather, to say that it cannot be an *essential* precondition of discovery.

2.4 Taking Stock

In this section, we presented what we take to be the most common way to think about what is required for someone to count as having made a discovery. This quotidian *Cognitivist* view turns on the very natural idea that, because genuine scientific discoveries are hard to come by, and difficult to predict, they must depend in some essential way on the cognitive capacities of the discoverer. Indeed, attending to many cases from the history of science suggests the view readily. But, we think that this view is mistaken. As we have shown, it struggles to make sense of clear cases of discovery. Moreover, as we will show in §3, it leads to the wrong conclusions concerning recent AI guided discoveries. As a result, while the line of thinking centered on cognitive capacities is certainly intuitive and seems, on the whole, to do an adequate job of identifying discoverers, its shortcomings give us strong reason to suspect that the correct view is to be found elsewhere.

3 AI Discovery

In this section we present two cases of AI scientific contributions, one extant, one imagined (but plausibly near) which we think merit the title of discoveries. Reflection on these cases will help us see where the Cognitivist approach goes awry and point toward a promising alternative.

3.1 Bin Packing Heuristics

One class of interesting and challenging problem in combinatorics is known as the *Bin Packing* problem. Bin packing involves ‘packing’ a collection of items $I = (i_1, i_2, \dots, i_n)$ of varying sizes $s(i_j)$ in the fewest number of bins B with a fixed total capacity C such that $\sum_{i \in B_k} s(i) \leq C$. The bin packing problem has two main variants, each presenting their own mathematically interesting challenges. *Offline* bin packing involves making packing decisions in a case where the sizes and packing order of all items are known in advance. In this variant, the optimal solution can, in principle, be found by exhaustive search over possible packings. In general, however, we do not have an efficient analytic method for doing so. Also brute-force solutions are infeasible for large I as the problem is NP-hard.

Online bin packing requires items of varying sizes to be packed one by one without knowledge of future items. In this case, the optimal solution for the full sequence is not available to the solver in the sense that the solver cannot, even in principle, access it in real time as, at any given moment, the solution space is not yet fully defined. The distinction between the two variants can be seen as the difference between computational hardness, on the one hand, and informational blindness, on the other, with the latter being more akin to scientific, empirical investigation than the former. As a result, in the online case, the best decision procedure for how to pack the next item in the online variant is necessarily heuristic with the two dominant approaches being ‘First-Fit’ and ‘Best-Fit’.

For the online case, the two dominant heuristics work as follows. Given an item i_j , let rC_k denote the remaining capacity of bin B_k . The first-fit heuristic places i_j into the first bin (that with the smallest index k) such that $s(i_j) \leq rC_k$. If no such bin exists, open a new bin. The best-fit heuristic is a bit more complicated and places i_j in the bin where the capacity of that bin after placement is minimized. More precisely, let $\mathcal{F} = k | s(i_j) \leq rC_k$ be the set of feasible bins and pack i_j into $k' \in \mathcal{F}$ such that $rC_{k'} - s(i_j) = \min_{k \in \mathcal{F}} (rC_k - s(i_j))$, and if \mathcal{F} is the empty set then open a new bin. The first-fit and best-fit heuristics achieve the best-known balance between worst-case theoretical guarantees and practical, empirical performance. While algorithms with lower, theoretical worst-case bounds are known, these tend not to perform better on average in practice. As a result of this balance of concerns, first-fit and best-fit are the most dominant known heuristics.

In [RPBN⁺24], researchers designed an AI based approach in an effort to surface a novel heuristic that could outperform first-fit and best-fit on average-case empirical performance. The approach centers on the design of a evolutionary computational framework that organizes the following elements. A large language model built on PaLM2 [ADF⁺23] (endearingly named `Codey`) that is fine-tuned on a large corpus of computer code. The model itself is not specifically designed to work on problems in mathematics and is not fine-tuned on mathematics specific texts. To check and score proposed heuristics, the framework also includes an evaluator function called `evaluate()`. Specifically, `evaluate()` checks whether a complete sequence of items has been packed into bins without exceeding their individual capacities. If the complete packing is valid, `evaluate()` assigns a numerical score equal to the negative of the number of bins used (so that scores closer to zero correspond to higher scores). Finally, the framework maintains a database in which candidate heuristics are stored, clustered, and sampled from in future cycles, while invalid or non-executing programs are discarded.

The framework evolves candidate heuristics as follows. The LLM is passed a Python program containing an empty function called `solve(item, bins)` which takes, as

input, an sized item $s(i_j)$ and an array of open bins and their current capacities. `solve()` governs the online packing process by deciding, for each arriving item, into which bin it should be placed. The LLM is prompted to generate code for a second function called `heuristic()`, which, given an item and a vector of remaining bin capacities, assigns a numerical score to each bin reflecting the desirability of placing the item there. Once the new `heuristic()` function is composed into the complete program, it is executed to simulate the packing of a benchmark sequence of items by repeatedly calling `solve()`. At the end of this process, `evaluate()` checks whether all items are validly packed and then scores the heuristic. `heuristic()` functions with valid packings and higher scores are stored in the database. This cycle (from the input of a skeleton to the generation of a candidate `heuristic()` function, to the evaluation of the resulting packing program, and the storage of those that do not violate bin capacity) constitutes a single pass of the algorithm.

On subsequent passes, high-scoring programs are sampled at random from the framework’s database and included in the input context to the LLM, which is prompted to improve the `heuristic()` function given the prior examples provided (in a manner similar to asking an LLM to improve ones writing). The framework then cycles through the process roughly 10^6 times until no further progress in improving `heuristic()` is made. The final heuristics are then evaluated on standard OR-Library benchmarks [Bea90] and synthetic Weibull-distributed instances [CDCO12], where performance is reported as the average fraction of excess bins used relative to the lower bound on the optimal offline solution.

Remarkably, the framework evolves a novel heuristic \mathcal{H}^* that had not been previously considered. It works by introducing a further consideration of the bin that would be selected by best-fit. For each new item $s(i_j)$, \mathcal{H}^* first assigns each feasible bin a score S_k by applying a ‘learned’ scoring function. Next, it applies best-fit, and then updates the score S_j of the bin B_j selected by the best-fit heuristic by applying $S_j^* = S_j \cdot s(i_j) - (rC_j - s(i_j))^4$. After this update, the heuristic then considers the scores of all bins (including the updated score S_j^*) and places the item in the bin with the highest score. The result is a heuristic that tends to pack items tightly but not *too tightly*, thereby avoiding the creation of small unusable gaps.

Claim: It is entirely apt to attribute discovery of \mathcal{H}^* to the AI system implementing this framework. Certainly, human scientists may have been in a position to validate the discovery of the heuristic in much the same way Bell Burnell’s discovery of PSR B1919+21 was validated. Still, in no less the way that Bell Burnell discovered PSR B1919+21, did the AI system here discover \mathcal{H}^* . Moreover, on the *Cognitivist* approach, it is not clear how to attribute discovery at all. It would be as if \mathcal{H}^* simply appeared.

Reflection: The framework described here did not involve any meta-reflective aware-

ness of its competences, let alone general mathematical competence. It certainly did not involve domain-general understanding. And yet, it discovers.

3.2 Future AlphaFold

Consider the following future potentially successful implementation of the neural network based program: *Future AlphaFold*. AlphaFold predicts the structure of proteins on the basis of their amino acid sequence [JEP⁺21b]. Imagine AlphaFold successfully predicting the structures of three proteins with a very different structure than current human-based techniques are able to map: P1, P2, and P3. As it turns out, the accurate mapping of P2's structure becomes crucial in a futuristic drug to cure hair-loss: *Moneymaker*.[△] Indeed, part of the cheap development costs of *Moneymaker* were that, without human intervention, it took the predicted structure output by AlphaFold and via an automated process of drug-design, built a drug around it.

Claim: It seems entirely apt, in describing the development of *Moneymaker*, to highlight the importance of the discovery of the structure of P2. Indeed, such a discovery-attribution seems perfectly felicitous. Imagine having a time-traveling friend tell you about the future of hair-loss science: “*Moneymaker* was developed by MegaCorp. They used the discovery of P2 which will happen in about three decades, so get a toupee which lasts until then.” Intuitions about the aptness of such a discovery-attribution are crystal clear. Indeed, it would be stilted to claim that scientists now possess or can now manipulate the structure of P2, but that it remains undiscovered or wasn’t the subject of a discovery. If ever discovery-attributions were warranted, they are so in the case of P2. Moreover, it would be a mistake to claim that P2 was resolved simply by ‘turning the crank’. After all, we can stipulate, no one knows or understands the principles and mechanisms relevant to predicting the folding of *any* of these proteins, P2 included. This is not, then, a simple case of simulation or mechanical verification.

Reflections: AlphaFold as described in its discovery of the structure of P2 fails to meet *Competence Principle*. It also fails any meta-reflective principle or domain general understanding.

Thus, AlphaFold fails to possess any of the purportedly necessary cognitive capaci-

[△]Future AlphaFold’s output is a prediction of a structure. Does this mean it cannot constitute a discovery? We think not. Consider the 2013 Nobel Prize in Physics. Here the award was given to François Englert and Peter Higgs for the “theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN’s Large Hadron Collider.” The prediction (here is a mechanism that would explain these results) is itself credited as a discovery as is the empirical verification of the phenomenon. While discoveries may need to be accurate or true, that they are in a sense a prediction needn’t impugn such status. Furthermore, we can tinker with the imagined case to generate a different output without affecting the arguments below.

ties for discovery. Yet, attributing it the discovery of P2's structure is perfectly apt. The description offered by your hair-conscious friend is entirely felicitous. Circumlocution to describe the case in terms of anything other than a discovery is, as noted, stilted and awkward. It would be improper to assert: "P2's structure was found and contributed to the development of *Moneymaker* but P2's structure was not discovered." We take this as strong evidence that none of these proposed missing capacities is strictly necessary for scientific discovery.

4 Navigating Epistemic Gaps

Let us take stock, we have argued that cases of human scientific discovery and AI discovery reveal that cognitive capacities of the sort under consideration, while exceedingly common, are not *essential*. So what is?

A genuine scientific discovery is an epistemic achievement. It is thus natural to suspect that the exercise of relevant cognitive capacities on the part of a discoverer is essential in discovery. But, this is to conflate aims with means. Rather, achievement of discovery is conceptually independent of the means by which it is achieved. To conflate the two is to mistake a contingent causal pathway for a constitutive condition. Instead, we propose, we should recognize discoverers as those who realize two kinds of epistemic achievement:

The Gap Spanning Proposal: to recognize a discoverer is to recognize their *success* in spanning epistemic gaps. Specifically, a discoverer is one whose work succeeds in *revealing* an epistemic gap, or succeeds in *bridging* an epistemic gap. Discovery is the successful spanning of an epistemic gap.

We think that this is a credible alternative to the view detailed in §2 because it succeeds in correctly classifying all of the cases that a Cognitivist approach gets right. It also correctly classifies cases like Pulsar, Bin Packing, and Future Alphafold. Let us explain.

Gap revealing discoveries are those episodes in science that bring to light anomalous or unexpected phenomena, thereby exposing a gap between what existing knowledge, theory, and expectations can accommodate and what is in fact observed. *Gap spanning* occurs when a previously revealed and well defined gap is filled by new knowledge, theory, or method. To attribute a discovery to someone (or something), it must be apt to say that their behavior *succeeded* in either revealing or spanning such an epistemic gap.

It is clear that what will be beneficial for producing discoveries in either mode will be a function of many complex factors: the mapping of the relevant problem space,

the maturity of the relevant science, whether the pertinent questions are “sharper” or “softer”, more or less amenable to the extant methods and tools of the scientific community [KM]. What counts as a genuine gap to be navigated will, we suspect, depend on our theoretical interests in classifying some episode in science as a discovery. Still, we think this approach preserves the ideas that discoveries in science constitute meaningful progress, that they are among the crucial drivers of scientific change. Scientists who make discoveries deserve important forms of credit and praise. They do so because they have successfully navigated a hitherto unbridged, unacknowledged, or unknown epistemic gap. Proof of concept here, however, will be in the pudding. And, indeed, we can recognize that our approach does well with the cases we have already considered.

For instance, we recognize Daeschler, Shubin, and Jenkins as having discovered *Tiktaalik* because their work succeeded in bridging a clearly defined gap in our understanding of the evolutionary transition from sea to land. At the same time, we do not recognize the Lintong farmers as having discovered the Terracotta Army because it is not appropriate to say that their actions *succeeded* in revealing or spanning an epistemic gap. Rather, their farming activity inadvertently or accidentally exposed an artifact. Subsequent archaeological inquiry revealed the first instance of this funerary practice which required accommodation by the best accounts of the Qin dynasty’s cultural practices. In [BG25], Bergamaschi Ganapini considers an analogous case in which a Roman child fell through a hole on the site of Nero’s ancient palace Domus Aurea. On our account, the child did not discover Domus Aurea, not because he lacked or failed to exercise relevant competencies, but simply because randomly falling through a hole does not count as a success at revealing or spanning a gap in our knowledge.

And, so, in this way the our view also supplies the conceptual resources for distinguishing between *luck* and *serendipity* [Cop]. Bell Burnell’s discovery of the pulsar was properly serendipitous. Hewish could have assigned another student to monitor that region of the northern sky. Nevertheless, it was Jocelyn who noticed the irregularity in the chart recorder’s input trend, and her response to that irregularity, focusing additional data gathering resources on that faint region of Vulpecula, that succeeded in revealing a gap in our astrophysical knowledge.

Crucially, both Bin Packing and Future AlphaFold involve the successful negotiation of epistemic gaps. Both of these cases involve AI intervention on a well-specified problem: bin-packing heuristic development and protein folding prediction respectively. In the case of Bin Packing, mathematicians knew that there must be better heuristics. But, they did not know what they were. The LLM powered framework discovers how to span that gap. This also explains why the polymerase chain reaction’s (PCR) technique and mere calculators, despite arriving at previously unknown results, are not discoverers. Unlike AI systems in these cases, a PCR or calculator constitute relevant

experimental and computational methods which help expedite the search for solutions to problems that we in principle can already secure. By contrast, the AI systems as described in Bin Packing and Future AlphaFold help *span* relevant epistemic gaps (to a better heuristic, or the structure of P2) in their respective and genuine discoveries. They figured out how to do so in a way that a PCR or calculator could not. We take this as evidence in favor of our proposed understanding of scientific discovery as well as another reason to reject the Cognitivist approach.

Still, some might feel hesitation at attributing to AI systems successful discoveries for reasons other than any lack of capacities.

5 Social Standing and Discovery?

We've argued that none of the purportedly missing capacities adduced by the Cognitivist approach are actually essential features of scientific discovery. Moreover, our central cases involve perfectly appropriate and felicitous attributions of discovery to AI systems. Accordingly, we claim, AI systems stand to make genuine scientific discoveries. But, this does not mean we think the bar for AI discovery is routinely met nor that the Cognitivist offers the only reasons for doubting the possibility of AI discovery.

In discussing these arguments with practicing scientists and theorists of science, we have encountered push-back in the form of appeals to a *social dimension* to discovery attributions. The thought is that discovery in science may require a certain kind of social standing and uptake. In principle form:

Standing Principle: For subject (or group) S' finding F of object Y to count as a scientific discovery of Y, S must have the appropriate standing to present F to the relevant scientific community.

Standing Principle can be unpacked in a number of different ways. The appropriate standing may be a function of one's epistemic capacities: recognized as the kind of inquirer who merits trust or reliance [Mac25, Due22].[△] Alternatively, appropriate standing might be cashed out by appeal to participation in the relevant social practices: participation in a practice of giving and asking for reasons [Bra94], or shared inquiry [Fria], say. Or it might involve institutional recognition: possessing the right kinds of institutional credentials to be deemed in good standing. Alternative proposals (and their combinations) abound.

Whichever way one understands *Standing Principle*, the worry, as we understand it, is that AI systems won't possess standing of the right sort to make discoveries,

[△]Of course, a position which takes standing as turning on possession of the capacities the Cognitivist adduced reduces to the position rejected in §2.

irrespective of their capacities. Accordingly, while this line of objection will grant that our arguments highlight the defects of the Cognitivist’s arguments, the worry is that our arguments fail ultimately to vindicate the possibility of AI discovery. As a result, it is simply the authors of Bin Packing that discovered the novel heuristic; the designers of Future Alphafold who discovered P2’s structure.

In response, we should note the dialectical force and intuitive power of our examples. We think they plausibly demonstrate that any such standing requirement is not necessary for discovery. Still, to avoid merely trading intuitions and to ensure our disagreement targets the same phenomenon, we opt for more direct engagement with this worry.

One strategy to take here would be to argue against the centrality of *Standing Principle* to an account of discovery. Such cases are possible to envision, perhaps as variation on the famous discovery of Ignaz Semmelweis, for instance. Semmelweis noted the increased rates of puerperal fever and subsequent death among women in the maternity ward. After careful inquiry, Semmelweis discovered that hand-washing helped reduce the spread of particles which gave rise to the fever. Semmelweis’s discovery and subsequent ameliorative efforts, however, were not well-received by the scientific community at the time. His work received little uptake, he was ostracized and ended up dying in a mental asylum in his late 40’s.

A counterexample to *Standing Principle* would involve a discoverer entirely outside the scientific community with, accordingly, no relevant social standing. It would then proceed along much the same lines as Semmelweis’s tragic tale: a discovery made but discredited. It seems clear such cases are possible and involve genuine discoveries.

The strategy we are inclined towards, however is more conciliatory. Insofar as it matters to attributions of discovery that the discoverer possesses appropriate standing, however that is to be cashed out, it is likely very many AI systems fail to meet that bar. Perhaps AI systems working in tandem with human scientists in a form of shared inquiry may prove the better subject of discovery [Frib, TNBM⁺]. Perhaps it is always a collective who is the correct locus of discovery, and sometimes for some purposes AI systems are part of the appropriate collective [CK22]. We grant, however, that extant AI systems will typically fail to meet *Standing Principle*.

Still, how long should this be the case? Is this really a crucial feature of scientific practice worth preserving? After all, the character of much scientific practice is shifting, and has shifted greatly since the Enlightenment. If the barrier to recognizing AI systems as capable of genuine scientific discovery is simply according them such standing, for how long should it be withheld? Again, this is not to say that we believe AIs should be viewed as scientists or awarded Nobel Prizes. But, rather, to acknowledge that, in cases like Bin Packing, the actual gap-spanning, the working out of and discovery of the novel online bin-packing heuristic, is due to the LLM precisely because the human authors

of the paper could not have gotten there alone. Accordingly, what principled reasons exist to withhold the standing necessary to credit such contributions as discoveries?

We suspect very few. As we've noted, AI systems in our examples are capable of making critical epistemic contributions which drive scientific change. For most any specification of the obstacle to being accorded appropriate status, it seems plausible future AI systems will meet it.^Δ The role AI systems play in scientific progress will likely only become further entrenched [DBPK⁺, RBX⁺]. If AI systems make core contributions, possess the internal capacities for making scientific discoveries, and are only unable to discover because of a failure to attribute to them a specific standing, why not attribute it?

The story would be different if AI systems failed to otherwise possess capacities necessary for scientific discovery. We've argued against that possibility above. It remains open that there are additional features of scientific discovery we have not highlighted, of course. Still, AI systems can (and certainly will) clearly play the relevant gap navigating roles we claim are central to discovery. Insofar as our negative arguments are successful, and on the basis of intuitions about cases like the ones we've offered, the proposed obstacle to AI scientific discovery would simply be meeting *Standing Principle*. This strikes us as a socially and historically contingent barrier, one which does not derive from the deepest features of science's epistemic credentials. Even if we grant to our opponent that some important social standing prevents AI systems from making discoveries now, the balance of reasons, we contend, will soon tip in the direction of according AI systems such status.

6 Reflection

Reflection on the possibility of AI discovery has led to a rejection of the necessity of the missing capacities adduced by the Cognitivist, and an alternative gap-negotiation approach to recognizing discoverers. Such reflection affords another opportunity to now isolate the work those purportedly missing capacities might perform. That is, each of the missing capacities we rejected was plausible to hold, present in, and meaningful contributor to many cases of scientific discovery. Is this merely a coincidence? Are these features purely vestigial remnants of an antiquated science? We think not.

Here we sketch important functions each of these capacities plausibly plays in human science. Even if these capacities aren't central features of scientific discovery, the functions they play are important in scientific practice and any future science must accommodate them.

^ΔTo take one example, advances in "agentic AI" highlight just how capably self-directed and even meaningfully autonomous such systems are becoming [Dun24]. If something like that is the barrier to being accorded appropriate standing, it seems like it will be soon surmounted.

Consider the demand that in manifesting competence a scientist can explain (provided some crucial background information) the relevance of her contribution. This would be a useful demand for a decentralized scientific practice in which sorting the epistemic wheat from the chaff is left in the first to practicing scientists themselves. Rather than rely solely on the expertise of others to assess the significance of a contribution, the burden is placed on the putative discoverer to assess how meaningful the contribution here stands to be. Requiring the ability to explain the significance of one's putative discovery stands to prove congenial to efficient resource distribution. It (alongside norms punishing free-riding) means an important barrier must already be reached for the broader scientific community to devote its resources to investigating and integrating a claim.

Furthermore, requiring such explanatory competence will plausibly play an important signaling role. If I can reliably highlight that this contribution, *qua* discovery, advances the state of understanding in a substantial way, I can help signal where further resources should be deployed and where further inquiring efforts should be conducted.

Similar morals apply to competence with standard reasoning processes in a domain. Scientific disciplines are epistemic practices subject to, among other things, their own internal norms and standards of appropriate methods of inquiry. Noting that meaningful contributions (discoveries) have been arrived at via the standard methods of that practice (competence) indicates that the standards of the discipline are conducive to progress [Fle25].

A meta-reflective principle plays a similar function. Requiring the skillful deployment of one's competence in a problem space means scientists will be better able to ascertain which first-order capacities are actually conducive to progress. As a result, further resources and training can be devoted to developing and refining those capacities/methodologies as opposed to others. Indeed, recognition of the successful application of capacities in a problem-space also highlights further the potential fecundity of such capacities to other problem-spaces. Furthermore, the skillful deployment of certain capacities highlights the ingenuity of particular scientists. Appending such a notion to discovery may serve to signal that particular scientists, and not just particular capacities, are worthy of further investment and attention.

Finally a domain-generality constraint plays a regulative role. Insofar as domain-general understanding is crucial to a putative discovery, this serves to reinforce the idea that prevailing scientific understanding in the domain writ large, as opposed to just one small area of it, is roughly on the right track. The fecundity of domain general-understanding serves as a corrective against worries that scientific progress is artificially specialized and narrow. If general understanding usefully serves discovery *here*, it cannot be so far off the mark all together.

Again, we stress that these functions are not necessary features of scientific discovery. Still, the signaling, allocative, and regulative roles we've sketched above seem part and parcel of a healthy scientific ecosystem. Transitioning to self-driving laboratories of the future need not jeopardize the centrality of discovery in science. For any such transition to prove successful, however, institutional mechanisms to realize the functions described above must also be developed.

7 Conclusion

Scientific practice stands ready to further incorporate AI systems. We've argued that despite recent resistance, many AI systems should be recognized as capable of making important scientific discoveries. From this emerges a conception of scientific discovery as involving the successful navigation of epistemic gaps. There is much more to say to develop this understanding of scientific discovery into a full-fledged account. It has helped here, however, to strip away non-essential capacities from the notion of discovery as remnants from a scientific practice engaged in solely by human agents. Nevertheless, these capacities, while non-essential, still help realize important functions in scientific practice.

The upshots of our arguments are three-fold. First, transitioning to AI-driven science should not be primarily a question of cognitive capacities. AI systems can or will realize the core functions of meaningful scientific contributors. The focus, instead, should shift to how to develop such systems appropriately and how best to deploy them. Second, we've isolated particular functions that the institution of science ought to ensure continue to be realized amid such a transition. If discovery-attributions will fail to be the appropriate vehicle for the realization of such functions, other mechanisms must be developed to compensate. The shape and structure of these features of institutional life may vary, but their role-specification is clear. These are both tasks that, we suspect, will best be addressed via collaboration between practicing scientists, technologists, and philosophers.

Finally, we take the forgoing arguments as illustrative of a broader methodological moral. The nature of the scientific enterprise stands on the precipice of dramatic change. Successful development and increased deployment of AI systems in science cannot be dismissed. As theoreticians and practitioners alike confront and navigate the increasingly non-human character of science, the centrality of familiar scientific commitments and concepts will be met with friction as they sit uncomfortably with successful practice. This friction will demand clear reflection on and substantial reconception of the nature and centrality of these commitments and concepts. Such friction will often allow us to isolate, expose, and refine our conception of the nature of genuine

epistemic progress in science, as well as to discern the functions played by irreducibly human elements of the scientific enterprise. Open consideration of the nature of mixed human-AI science will lend itself to important reconception of crucial scientific concepts and core commitments [ED25]. Rather than resist such reconception, we hope to have shown the theoretical import of embracing it.

References

- [ADF⁺23] Rohan Anil, Andrew M Dai, Orhan Firat, Melvin Johnson, Dmitry Lepikhin, Alexandre Passos, Siamak Shakeri, Emanuel Taropa, Paige Bailey, Zhifeng Chen, et al. Palm 2 technical report. *arXiv preprint arXiv:2305.10403*, 2023.
- [Bea90] John E Beasley. Or-library: distributing test problems by electronic mail. *Journal of the operational research society*, 41(11):1069–1072, 1990.
- [BG25] Marianna Bergamaschi Ganapini. Can ai make scientific discoveries? *Philosophical Studies*, pages 1–19, 2025.
- [Bog21] Florian J Boge. Two dimensions of opacity and the deep learning predicament. *Minds and Machines*, pages 1–33, 2021.
- [Bra94] Robert Brandom. *Making It Explicit: Reasoning, Representing, and Discursive Commitment*. Harvard University Press, Cambridge, Mass., 1994.
- [CDCO12] Ignacio Castiñeiras, Milan De Cauwer, and Barry O’Sullivan. Weibull-based benchmarks for bin packing. In *International Conference on Principles and Practice of Constraint Programming*, pages 207–222. Springer, 2012.
- [Cet99] Karin Knorr Cetina. *Epistemic cultures: How the sciences make knowledge*. harvard university press, 1999.
- [CK22] Elinor Clark and Donal Khosrowi. Decentring the discoverer: How AI helps us rethink scientific discovery. *Synthese*, 200(6):463, 2022.
- [Cop] Samantha Copeland. On Serendipity in Science: Discovery at the Intersection of Chance and Wisdom. 6:1–22.
- [Cra20] George Crabtree. Self-Driving Laboratories Coming of Age. *Joule*, 4(12):2538–2541, 2020. Publisher: Elsevier.
- [Cre20] Kathleen A Creel. Transparency in complex computational systems. *Philosophy of Science*, 87(4):568–589, 2020.

[DBPK⁺] Fatih Dinc, Marta Blanco-Pozo, David Klindt, Francisco Acosta, Yiqi Jiang, Sadegh Ebrahimi, Adam Shai, Hidenori Tanaka, Peng Yuan, Mark J. Schnitzer, and Nina Miolane. Latent computing by biological neural networks: A dynamical systems framework.

[DSJJ06] Edward B Daeschler, Neil H Shubin, and Farish A Jenkins Jr. A devonian tetrapod-like fish and the evolution of the tetrapod body plan. *Nature*, 440(7085):757–763, 2006.

[Due22] Eamon Duede. Instruments, agents, and artificial intelligence: novel epistemic categories of reliability. *Synthese*, 200(6):491, 2022.

[Due23] Eamon Duede. Deep learning opacity in scientific discovery. *Philosophy of Science*, 90(5):1089–1099, 2023. Publisher: Cambridge University Press.

[Dun97] Kevin Dunbar. How scientists think: On-line creativity and conceptual change in science. 1997.

[Dun24] Leonard Dung. Understanding Artificial Agency. *The Philosophical Quarterly*, page pqae010, February 2024.

[DVB⁺21] Alex Davies, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, et al. Advancing mathematics by guiding human intuition with ai. *Nature*, 600(7887):70–74, 2021.

[ED25] James Evans and Eamon Duede. After science. *Science*, 390(6774), 2025.

[Fey93] Paul Feyerabend. *Against Method*. New Left Books, London, 1993.

[Fle25] Will Fleisher. Epistemic Practices: A unified account of epistemic and zetetic normativity. *Noûs*, 59(1):289–314, 2025.

[Fria] Daniel C. Friedman. Cooperation and Shared Inquiry. *Australasian Journal of Philosophy*.

[Frib] Daniel C. Friedman. Embracing HAL: Artificial Joint Inquiry. MS.

[GBAIH⁺16] Rafael Gómez-Bombarelli, Jorge Aguilera-Iparraguirre, Timothy D Hirzel, David Duvenaud, Dougal Maclaurin, Martin A Blood-Forsythe, Hyun Sik Chae, Markus Einzinger, Dong-Gwang Ha, Tony Wu, Georgios Markopoulos, Soonok Jeon, Hosuk Kang, Hiroshi Miyazaki, Masaki Numata, Sunghan Kim, Wenliang Huang, Seong Ik Hong, Marc Baldo, Ryan P. Adams, and Alán Aspuru-Guzik. Design of efficient molecular

organic light-emitting diodes by a high-throughput virtual screening and experimental approach. *Nature Materials*, 15(10):1120–1127, 2016.

[Hal21] Marta Halina. Insightful artificial intelligence. *Mind & Language*, 36(2):315–329, 2021. _eprint: <https://onlinelibrary.wiley.com/doi/pdf/10.1111/mila.12321>.

[HBP⁺68] Antony Hewish, S. Jocelyn Bell, John D. H. Pilkington, Paul F. Scott, and Robin A. Collins. Observation of a rapidly pulsating radio source. *Nature*, 217(5130):709–713, February 1968.

[Her24] John Herschel. Preliminary discourse on the study of natural philosophy. In *Literature and Science, 1660-1834, Part II vol 6*, pages 391–410. Routledge, 2024.

[JEP⁺21a] John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, et al. Highly accurate protein structure prediction with alphafold. *nature*, 596(7873):583–589, 2021.

[JEP⁺21b] John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishabh Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, Martin Steinegger, Michalina Pacholska, Tamas Berghammer, Sebastian Bodenstein, David Silver, Oriol Vinyals, Andrew W. Senior, Koray Kavukcuoglu, Pushmeet Kohli, and Demis Hassabis. Highly accurate protein structure prediction with AlphaFold. *Nature*, 596(7873):583–589, August 2021. Publisher: Nature Publishing Group.

[KM] Kareem Khalifa and Jared Millson. Inquiry and Underdetermination. In Aaron B. Crelle and Jonathan Matheson, editors, *Inquiry: Philosophical Perspectives*, pages 236–253. Routledge.

[KTE19] Austin C Kozlowski, Matt Taddy, and James A Evans. The geometry of culture: Analyzing the meanings of class through word embeddings. *American Sociological Review*, 84(5):905–949, 2019.

[Kuh97] Thomas S Kuhn. *The structure of scientific revolutions*, volume 962. University of Chicago press Chicago, 1997.

[Led01] Lothar Ledderose. *Ten thousand things: module and mass production in Chinese art*. Princeton University Press, 2001.

[Mac25] Edouard Machery. Science Without Trust? *Philosophy of Science*, pages 1–13, August 2025.

[NSS62] Allen Newell, J Clifford Shaw, and Herbert A Simon. The processes of creative thinking. In *Contemporary Approaches to Creative Thinking*. Atherton Press, 1962.

[Pop34] Karl Raimund Popper. *The Logic of Scientific Discovery*. Routledge, New York, 1934.

[Pop14] Karl Popper. *Conjectures and refutations: The growth of scientific knowledge*. routledge, 2014.

[RBX⁺] Till Richter, Mojtaba Bahrami, Yufan Xia, David S. Fischer, and Fabian J. Theis. Delineating the effective use of self-supervised learning in single-cell genomics. pages 1–11.

[Rei38] Hans Reichenbach. Experience and prediction: An analysis of the foundations and the structure of knowledge. 1938.

[RPBN⁺24] Bernardino Romera-Paredes, Mohammadamin Barekatain, Alexander Novikov, Matej Balog, M Pawan Kumar, Emilien Dupont, Francisco JR Ruiz, Jordan S Ellenberg, Pengming Wang, Omar Fawzi, et al. Mathematical discoveries from program search with large language models. *Nature*, 625(7995):468–475, 2024.

[Sch25] Jutta Schickore. Scientific Discovery. In Edward N. Zalta and Uri Nodelman, editors, *The Stanford Encyclopedia of Philosophy*. Metaphysics Research Lab, Stanford University, Fall 2025 edition, 2025.

[Sim04] Dean Keith Simonton. *Creativity in science: Chance, logic, genius, and zeitgeist*. Cambridge University Press, 2004.

[Sos] Ernest Sosa. *A Virtue Epistemology: Apt Belief and Reflective Knowledge, Volume I*. Oxford University Press.

[Stu19] Michael T. Stuart. The Role of Imagination in Social Scientific Discovery: Why Machine Discoverers Will Need Imagination Algorithms. In Mark Addis, Peter C. R. Lane, Peter D. Sozou, and Fernand Gobet, editors, *Scientific Discovery in the Social Sciences*, volume 413, pages 49–66. Springer International Publishing, Cham, 2019. Series Title: Synthese Library.

[Sul19] Emily Sullivan. Understanding from machine learning models. *British Journal for the Philosophy of Science*, 2019.

[TDW⁺19] Vahe Tshitoyan, John Dagdelen, Leigh Weston, Alexander Dunn, Ziqin Rong, Olga Kononova, Kristin A Persson, Gerbrand Ceder, and Anubhav Jain. Unsupervised word embeddings capture latent knowledge from materials science literature. *Nature*, 571(7763):95–98, 2019.

[TNBM⁺] Alireza Tamaddoni-Nezhad, David A. Bohan, Ghazal Afrozzi Milani, Alan Raybould, and Stephen Muggleton. Human-machine scientific discovery. In *Human-Like Machine Intelligence*, pages 279–315. Oxford University Press.

[TWL⁺24] Trieu H Trinh, Yuhuai Wu, Quoc V Le, He He, and Thang Luong. Solving olympiad geometry without human demonstrations. *Nature*, 625(7995):476–482, 2024.

[Wal] Louise Walsh. Journeys of discovery: Jocelyn Bell Burnell and pulsars.

[Wan25] Dashun Wang. Prizes must recognize machine contributions to discovery. *Nature*, 646(8084):261, 2025.