

Prediction and discovery in the search for chemical elements¹

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Abstract

It has become increasingly difficult to discover new chemical elements. Whether this is because science approaches the endpoint of this endeavour or because of experimental limitations, this difficulty affects how we conceive two central concepts: element discovery and the periodic table's predictive power. First, I argue that the concept of element discovery has undergone a shift and that latest attempts to offer specific criteria for an element's discovery have rendered the concept flexible and fluid. Secondly, I argue that the way in which scientists try to discover elements beyond atomic number 118 shows that the periodic table no longer possesses the predictive power that is standardly associated with it. Therefore, we should construe differently what it means for the table to be predictively powerful.

1. Introduction

Predicting how things happen is one of the highest virtues of modern science. Prediction does not concern exclusively claims about the future. Paleontology makes predictions about animals and plants that existed millions of years ago. It can also concern things that are happening now but to which we have no direct observable access. For example, astrochemistry makes predictions about the chemical composition of the atmosphere of distant planets. In general, predictive claims are claims about objects, processes or phenomena that have not yet been sufficiently corroborated through reliable empirical means (or, to put it crudely, that we do not know yet) (e.g. Barrett and Kyle Stanford 2005).¹

Relatedly, scientific discovery is often associated with the idea of acquiring new insight into the object or phenomenon science is studying. It can take different forms; either refer to the discovery of an object (such as a planet, element or form of energy) or to the discovery of a previously unknown property or process (such as that the earth moves around the sun). What is important in cases of

¹ Preprint of chapter In *The Perils and Promises of Prediction: Historical and Epistemological Perspectives*, ed. By Theodore Arabatzis, Stathis Arapostathis, Iraklis Katsaloulis and Aristotle Tympas, Boston Studies in the Philosophy and History of Science. Cham: Springer Nature (In press)

¹ Of course, not all attempted predictions turn out to be correct: scientists have made predictions that were false. For example, Mendeleev falsely predicted that there exist two elements that are lighter than hydrogen (Scerri 2007: 140). I thank the reviewers for bringing this to my attention.

purported scientific discoveries is that they carry considerable epistemic weight in the following sense: when the scientific community proclaims to have discovered something, this discovery is not perceived as a conjecture but as an empirically well-established fact, namely as something that we have sufficient justification to believe in (put crudely again, that we know of).²

Scientific predictions and discoveries are connected as discoveries are often invoked as evidence that a prediction is correct (or not). Take for instance Neptune's discovery. When in 1821 Alexis Bouvard formulated astronomical tables for the orbit of Uranus based on Newton's laws of motion, astronomers noticed that the observational data for Uranus' position did not match with the predictions of Newton's theory. This led some astronomers to claim that there exists a planet which has not been discovered yet and which influences the orbit of Uranus. Indeed, this prediction of an unknown planet was corroborated with the discovery of Neptune in the mid 1800s by Urbain Le Verrier (and some say, independently by John Couch Adams).³ Note that while in this case the discovery of Neptune supported the prediction of Newton's theory, a discovery can also contradict one. This, for example, was the case with Mercury's orbit whose observed position deviated from the predictions of Newton's theory, eventually leading to its dismissal over Einstein's relativity theory.

In philosophy of science, the concepts of prediction and discovery have received considerable attention. Their investigation has been connected to major philosophical issues around science such as the nature of knowledge, scientific realism, confirmation, and the distinction between science and pseudoscience (e.g. Goodman 1983; Lakatos 1970; Popper 1959; Reichenbach 1938 to name just a few). Among the questions asked are: (i) how important are successful predictions to the confirmation of a theory; (ii) what are the main features of a scientific discovery; and (iii) what is the role of predictions in distinguishing science from pseudoscience?

This paper does not raise a philosophical question (of the aforementioned sort) with respect to discovery and prediction, but rather addresses a conceptual one. Specifically, it investigates how the concepts of prediction and discovery are construed in science with respect to chemical elements. The prediction and discovery of chemical elements has been and continues to be one of the most prestigious endeavours one can undertake. Once achieved, it receives notable recognition by the

² This does not mean that there have not been instances of proclaimed discoveries that later turned out to be false. One can find such examples in the history of element discovery (e.g. Fontani et al. 2015).

³ There were disputes about who should be granted priority as to the discovery, some even suggesting that Galileo had discovered it first (e.g. Drake and Kowal 1980; Smart 1947).

scientific community and the discoverer is granted the right to name the element.⁴ It is also one of the most exciting topics in the history of science, revealing valuable information about the practice of chemistry, but also stories of political, institutional and personal intrigue (e.g. Ball 2021; Scerri 2019).⁵

The paper maps how the prediction and discovery of elements have changed practically and, as a consequence, conceptually. First, it shows that what it means to discover elements is not the same today as it was in the past.⁶ The chemical community has proposed, revised and extended the criteria for acknowledging an element discovery, thus suggesting that the concept is best construed as fluid. Secondly, it argues that a shift in how we construe the periodic table's predictive power should also be made. This is because the periodic table is no longer predictively powerful in the way it has been standardly lauded for. So, unless one accepts that this is the end to the table's ability for predictions, we should revise how we construe the predictive power of the table.

Section 2 maps how the concept of element discovery has changed from referring to a process of finding and isolating chemical elements in nature, to synthesising very few unstable atoms in the laboratory. This change has led to the proposal of a flexible set of criteria for element discovery, thus suggesting that it should be construed as a fluid concept. Section 3 presents how prediction has changed with respect to chemical elements. Based on this, I claim that we should revise how we evaluate the predictive power of the periodic table. Section 4 concludes.

2. The changing meaning of element discovery

2.1 From finding elements to making them

The term 'element' has a long history, going back millennia and meaning different things.⁷ While I do not offer a complete historical overview of how this term has been construed, it is safe to say that initially and for a long time the term was connected by some civilisations to the idea that everything is made of a few fundamental constituents of matter. For example, in ancient China, it was believed

⁴ One can appreciate the prestige associated with elemental discovery by how the Nobel Foundation describes the recognition it places to pioneers in elemental discovery (<https://www.nobelprize.org/stories/pioneers-of-the-periodic-table/>).

⁵ These intrigues were often prompted by priority disputes about who discovered an element first or how it should be named.

⁶ This is not the only instance in science where this is noticed. For example, Allan Franklin (2018) discusses how the standards for discovery have changed with respect to particle physics.

⁷ This is a very brief and incomplete sketch of how elements were construed prior to the emergence of what we recognise today as modern chemistry (see below). Nuances and details that are important to an accurate historical reconstruction of this idea are not presented here.

that there are five elements: water, earth, metal, wood and fire. In ancient Greece, Empedocles- and later Aristotle- thought that there are four fundamental elements: water, earth, fire and air.⁸

This last idea, becoming part of the Aristotelian worldview, formed the basis of how the constitution and transformation of matter was understood and studied in alchemy, including by ancient Egyptian alchemists and extending to medieval alchemists in Western Europe (e.g. Principe 2012 for a historical overview of alchemy). Eventually some alchemists proposed changes as to which elements should be regarded fundamental and diverged from Aristotle's original worldview.⁹ Despite these divergences, in alchemy there was no question regarding the discovery of new elements as they were all considered to be known. Instead, what preoccupied alchemists was how to manipulate matter so as to extract and purify elements with the purpose to make the so-called Philosopher's Stone (or Elixir of Life) that would transmute metals (and possibly all matter) into gold.

This does not mean that elements were not discovered during that time. Alchemists managed to isolate what we recognise today as chemical elements such as antimony, arsenic and zinc. From our current perspective, these are considered examples of element discoveries even if they were not recognised as such by those who made them.

With the Scientific Revolution of the 16th and 17th centuries, modern science gradually takes the form which is now recognisable to us both in terms of its institutionalisation and in terms of its methods. In this context, chemistry emerged as a rigorous scientific discipline that is separate from the activities, questions and methods of alchemy, and dispensed with its mystical considerations (large credit to this break from alchemy is given to Robert Boyle).¹⁰ With respect to elements, the major conceptual turning point comes in the 18th century when Antoine-Laurent Lavoisier publishes the *Traité élémentaire de chimie*. In it, he offered what is nowadays regarded as the first

⁸ Admittedly, this is a very simplified presentation of the idea of elements (see e.g. Ball 2021; Brock 1992; Brown and Ladyman 2019)

⁹ For example, in the 16th century Paracelsus diverged from the accepted Aristotelian worldview within which alchemists worked and proposed that there are three fundamental elements: sulfur, salt and mercury.

¹⁰ Some historians are now challenging the perceived view that alchemy was completely separate from chemistry by revealing how alchemists developed important chemical methods and experiments, and contributed to the advancement of chemical knowledge (e.g. Newman and Principe 2010; Principe 2012). This issue is not discussed here.

definition of chemical elements.¹¹ Specifically, he defined elements as those substances that cannot be further decomposed by means of chemical analysis (Hendry 2005: 31).

By defining elements in terms of the final limit of analysis, Lavoisier established (even if unknowingly) three central parameters for a substance to act as the empirical basis for an element's discovery. First, the discovered substance had to be as pure as possible; there should not be any other chemical entities (elements, molecules, etc.) contained in it. Another way this is put, is by requiring the element (in the form of a pure substance) to be isolated from other chemical entities. Isolation could be achieved in different ways, including by means of electrolysis (for ex. see the discoveries of calcium, sodium and potassium), heating (for ex. see the discovery of oxygen), or reduction (for ex. see the discovery of manganese) (e.g. Ball 2021).

Secondly, the isolated substance which purportedly represented the discovery of an element had to stay relatively stable (under some set of conditions).¹² Given that chemists at the time had no knowledge of the nuclear structure of elements, stability should be taken here rather liberally to refer to both chemical and physical stability. That is, a pure substance should be relatively stable (under some conditions) with respect to chemical change as well as to nuclear decay, in order for chemists to be able to study and corroborate the properties of the newly discovered element.¹³

¹¹ There are disagreements about whether Lavoisier should be credited for being the first to define chemical elements this way. The idea that a "substance is viewed as elementary if it cannot be decomposed by the tools of the chymist" was purportedly formulated as early as the High Middle Ages (if not sooner) by alchemists (Newman 2011: 319). Boyle is also said to have expressed the same idea when defining elements as "those primitive and simple Bodies of which the mixt ones are said to be composed, and into which they are ultimately resolved" (quote from Boyle's *The Sceptical Chymist* in Hunter and Davies 1999: 220).

¹² Being *relatively* stable is determined by the experimental and technological means that the chemists had available at different times and which allowed them to observe and manipulate substances (see Seifert (forthcoming)).

¹³ An atom is the "(s)mallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge carrying almost all its mass and electrons determining its size" (IUPAC 2014: 121). A nucleus is "(t)he positively charged central portion of an atom, excluding the orbital electrons" (IUPAC 2014: 1019). It is constituted by a number of protons and neutrons. A nuclide is a "species of atom, characterized by its mass number, atomic number and nuclear energy state" (IUPAC 2014: 1020). Atomic number refers to the number of protons in the nuclide; mass number is the "(t)otal number of heavy particles (protons and neutrons jointly called nucleons) in the atomic nucleus" (IUPAC 2014: 885). Isotopes are "(n)uclides having the same atomic number but different mass numbers" (IUPAC 2014: 794).

The third parameter for element discovery which follows from the second and is revealed by the practical study of elements, is that the sample is of sufficient amount so as to be examinable. While to the present author's knowledge there was no explicit mention of what that proper amount is, fulfilling this parameter was essential so as to be able to study the chemical and physical properties of the discovered element (including of its boiling and melting point, its reactivity, and so on). That this was an important feature also becomes evident from the fact that later on, the difficulty to extract a good amount of the pure substance posed a serious challenge for admitting the discovery of an element (see below).

I should note that elements were discovered even prior to Lavoisier's definition and were hypothesised and predicted even if chemists had not (yet) achieved isolation of a stable amount of the relevant pure substance. However, Lavoisier's definition clarified the parameters of element discovery and thus established an empirical basis upon which chemists could decide (and agree) on whether a discovery of an element had been achieved or not.¹⁴

The second event which shaped chemistry's notion of element discovery was the acceptance of Mendeleev's proposed classification of chemical elements in 1869; namely of his periodic table.¹⁵ Lavoisier had already published a list of the known elements of his time, but in the 19th century chemists started to propose specific orderings of the chemical elements that would help them systematise and organise the knowledge they had acquired about them.¹⁶ While there were competing classifications initially proposed, Mendeleev's table was the one that was eventually accepted by the community (e.g. Pulkkinen 2020). In his proposed classification, chemical elements were ordered in terms of increasing atomic weight.¹⁷

What is relevant in the present analysis is that Mendeleev's table contained gaps, thus suggesting that there exist elements which have not been discovered yet. Moreover, certain patterns in the chemical and physical properties of sets of elements became much more apparent. The values of certain properties could be inferred by the position of the predicted element in the table. In the

¹⁴ I take Lavoisier's definition to establish an empirical- not conceptual- basis for elemental discovery because his definition is functional: it tells you when practically (in an experiment) you have reached the point where the examined sample corresponds to a pure substance. It does not tell you anything about the nature of chemical elements.

¹⁵ Obviously, I am disregarding other equally important episodes in the history of chemistry, including Dalton's postulation of atoms. I only focus on those episodes that I believe have had the largest effect on the concepts of element discovery and prediction.

¹⁶ Note that Lavoisier included in his list of elements things that scientists no longer recognise as such, such as light and caloric (Scerri 2007: 5). I thank the reviewers for bringing this to my attention.

¹⁷ Later on, Mendeleev's table was amended and the classification of elements was based on ordering them in terms of increasing atomic number. This is now the defining principle of the modern table.

modern form of the table (see footnote 17) this became even more apparent as elements are now grouped into multiple sets in the table (called groups, periods and families) based on specific properties they have in common.

All this helped chemists predict what sort of properties they should expect by those elements that had not been discovered yet. That is, Mendeleev's classification of elements and the use of his suggested table rendered the discovery of new chemical elements a more precise activity. The periodic table, with its empty gaps and predicted properties of elements, gave a much more precise direction regarding (i) which elements to look for; and, (ii) when chemists could confidently say (through the measurement of specific properties) to have discovered them. So, apart from exhausting all means of analysis with respect to a specific substance (as per Lavoisier's definition), a successful discovery also involved the measurement of specific properties (such as atomic weight, boiling point, reactivity, etc.) so as to decide whether what has been isolated is in fact a new element that fills a specific gap in the table, and exhibits the properties that are expected of it in virtue of its position in that table.

All this formed part of how chemists generally construed element discovery. Specifically, it is safe to infer from how element discovery was practically pursued that it was accepted (even if implicitly) that one would have to produce by some means of isolation a sufficient amount of relatively stable pure substance. Moreover, one should be able to produce empirical evidence that this pure substance possesses physical and chemical properties that are close to those predicted for the unknown elements posited by the periodic table.¹⁸

By the beginning of the 20th century, practical difficulties emerged that made it hard to fulfil these requirements for element discovery. It became very difficult to find new naturally occurring elements and whenever they were found and isolated, they were in very small quantities to study them. For example, when radium was discovered by Marie and Pierre Curie in 1898, they extracted only 1mg of that element from ten tons of uranium ore pitchblende. The turning point eventually came between 1925 and 1937, when rhenium and technetium were respectively discovered. This is how the Royal Society of Chemistry describes rhenium's discovery:

The periodic table had two vacant slots below manganese and finding these missing elements, technetium and rhenium, proved difficult. Rhenium was the lower one and indeed it was the last stable, non-radioactive, naturally-occurring element to be discovered. In 1905, Masataka Ogawa found it in the mineral thorianite from Sri Lanka. He realised from lines in

¹⁸ This does not mean that Mendeleev's initially proposed table did not make some failed predictions both with respect to predicted elements (as he falsely predicted- among other- two elements lighter than hydrogen) but also with respect to the properties of undiscovered elements (e.g. Scerri 2007: 140-143).

its atomic spectrum that it contained an unknown element. He wrongly thought it was the one directly below manganese and so his claim was discounted at the time. However, a re-examination of Ogawa's original photographic spectra proved he had discovered rhenium. The isolation of rhenium was finally achieved in May 1925 by Walter Noddack and Ida Tacke working in Berlin. They concentrated it from the ore gadolinite in which it was an impurity.¹⁹

Rhenium turned out to be the last element to be discovered by isolating it. The next element to be discovered - technetium - is the first element to be discovered not by some process of isolation but by synthesis. This is how the Royal Society recounts its discovery:

Technetium long tantalised chemists because it could not be found. We now know that all its isotopes are radioactive and any mineral deposits of the element had long disappeared from the Earth's crust. (The longest lived isotope has a half life of 4 million years.) Even so, some technetium atoms are produced as uranium undergoes nuclear fission and there is about 1 milligram of technetium in a tonne of uranium. Claims in the 1920s to have found this element, or at least to have observed its spectrum, cannot be entirely discounted. Technetium was discovered by Emilio Segrè in 1937 in Italy. He investigated molybdenum from California which had been exposed to high energy radiation and he found technetium to be present and separated it. Today, this element is extracted from spent nuclear fuel rods in tonne quantities.²⁰

From this point onwards, the elements are not found through some process of isolation, but via synthesis. This is because the new elements are either very difficult to find naturally, or do not exist at all on earth as they are highly unstable (in the sense of having a very short half-life).²¹ Another reason for chemists choosing to synthesise new elements is the development of technological means that allowed for it: most notably the cyclotron. The cyclotron is the result of the progress achieved in nuclear physics at the beginning of the 20th century. It was made in 1929-1930 by Ernest Lawrence and is a type of particle accelerator which bombards atomic nuclei with particles so as to create new elements.

All this suggests a shift in the meaning of element discovery. A discovery was no longer decided by achieving the isolation of a substantial amount of a relatively stable pure chemical substance which naturally occurs on earth. While extracting a new chemical element without impurities was still a desirable objective, isolating a substance from any impurities in a good amount and for a relatively proper amount of time, was no longer practically possible. These difficulties became even more

¹⁹ <https://www.rsc.org/periodic-table/element/75/rhenium>

²⁰ <https://www.rsc.org/periodic-table/element/43/technetium#history>

²¹ Here I am referring to nuclear stability.

apparent towards the end of the 20th century. By 1984, almost all seven rows of the periodic table were complete: the elements predicted by the table had almost all been discovered either in nature or by synthesising them, with only nine elements missing to complete the last row.

While this is a successful record of element discovery, it was not achieved without significant hurdles. From 1955 to 1984, there were instances of contradictory results regarding the discovery of elements with atomic numbers between 101 and 109. This led to controversies within the community, false claims as to the discovery of new elements, and priority disputes about who should be credited and allowed to choose the name of the new element.

The most notable example of these controversies are the so-called 'transfermium wars' which concerned priority disputes about the discovery of elements with atomic numbers of 101 to 109 (Sargeson et al. 1994). These disputes are partly explicable on extra-scientific grounds: it was, after all, the period of the cold war and among the competing research groups were those based in the USA and USSR. Nevertheless, a contributing factor for these problems was that element discovery had become very difficult to achieve in the way that it was initially established. Specifically, none of the initial three parameters of element discovery mentioned above could be maintained. First, it was not possible to isolate from nature a new pure substance. Secondly, even by means of synthesis, the newly discovered elements were rarely (if ever) stable. Rather the contrary, their half-lives could be as short as a few seconds (or less). Third, chemists could not synthesise sufficient amounts of the pure substance that would allow them to then study the new element's chemical and physical properties. In some instances, chemists would produce just very few atoms that would very quickly decay into lighter elements. These difficulties were later reported by the Transfermium Working Group:

The discovery (synthesis) of a new element has become a very complicated matter because it now requires the intricate equipment of nuclear physics and because the number of atoms prepared is often extremely small. The very short half-life of many of the isotopes poses still further problems of experimentation. There has been considerable discussion and some disagreement concerning the discovery of the transfermium elements. (Wapstra 1991: 880)

This led the community to an important institutional decision. Unless one wanted to admit that it is no longer possible to discover new elements, element discovery - together with its initially set empirical parameters- had to be revised. And so it happened. The 'transfermium wars' led the International Union for Pure and Applied Chemistry (IUPAC), together with the International Union for Pure and Applied Physics (IUPAP), to establish the Transfermium Working Group (TWG) which was assigned to produce two reports. The first report, titled 'Criteria that must be satisfied for the DISCOVERY OF A NEW CHEMICAL ELEMENT TO BE RECOGNIZED', establishes the criteria for a purported element discovery to be recognised as such (Wapstra 1991). The second report applies the criteria of the first to the case of the transfermium elements so as to resolve the

disputes around their discovery (Barber et al. 1993; see also Sargeson et. al. 1994). Regardless of whether and how these particular disputes were resolved, what is relevant to the present analysis is how they prompted for the first time an explicit effort by the chemical and physical community to (a) lay down the criteria by which something is deemed an element discovery; and (b) adjust the concept of element discovery to the practical limitations faced at the time.

Before presenting some of the criteria set for element discovery by the TWG, note that a need to amend the concept of element discovery is acknowledged in the 1991 report in the following way:

The TWG has had to adopt an historical perspective in establishing its criteria and testing them through the shadow exercises but, of course, the application of the criteria lies largely in the future. However, it is evident that, historically, new elements were proposed, and accepted, on the basis of evidence that would not meet the criteria of today, even prior to the codification upon which the TWG has been engaged. (..) The standards of the times have markedly tightened, not least because of the development of new experimental technologies and, particularly, of the computer. (Wapstra 1991: 882)

The report presents eight criteria that an element discovery should meet. I do not present them in full but rather focus on those that show the extent to which the concept of element discovery has changed compared to how it was initially thought. Specifically, I focus on criteria II.1 and II.6.

Criterion II.1 gives the definition of discovery: “(d)iscovery of a chemical element is the experimental demonstration, beyond reasonable doubt, of the existence of a nuclide with an atomic number Z not identified before, existing for at least 10^{-14} s” (Wapstra 1991: 883). This criterion is informative as to the following. First, the range of accepted stability for a newly discovered element is (i) significantly small; but also (ii) specified quantitatively for the first time. Secondly, that a sufficient amount of sample is discovered (i.e. synthesised) is not considered a requirement for the successful discovery of an element. This is shown by the criterion’s reference to just one nuclide in the definition of discovery, as well as by Note 1 which states that “(t)his lifetime is chosen as a reasonable estimate of the time it takes for a nucleus to acquire its outer electrons” (Wapstra 1991: 883). Both quotations suggest that a discovery could involve just a single nuclide.

Criterion II.6 talks of chemical purification. It states that in cases where the presence and influence of impurities in the new elements can be recognised and explained, then the relevant methods employed for the synthesis of these elements are deemed acceptable. In other cases where “a nuclide is obtained by chemically purifying natural material or debris of (thermo-)nuclear explosions”, methods to purify the nuclides are required (Wapstra 1991: 884). Overall, it seems that purity is still an important parameter to element discovery, though in a more lenient manner if the presence of impurities is explicable.

In conclusion, the fact that the chemical community was prompted to acknowledge the need to precisify the concept of element discovery is suggestive of its conceptual change. The criteria that were set- for the first time- for element discovery show how the role of previously central features to it (namely of stability, sufficient amount, and purity) has now either been restricted or discarded. Section 2.2 shows that the proposal of specific criteria (in the form offered by TWG 's report) instead of rendering the concept of element discovery more precise, actually led to the formation of a more fluid and flexible concept.

2.2 The fluidity of the concept of element discovery

Even though the 1991 report of the TWG offered for the first time a widely accepted, institutionally approved set of criteria for element discovery, a closer look at that report as well as of the revised one which was produced in 2018 by a new working group (called the Joint Working Group, JWG) reveal that the scientific community is starting to adopt a much more flexible and fluid concept of element discovery. Let me explain in what sense.

First, the 1991 report of the TWG points out that its proposed criteria should not be viewed as either necessary or sufficient for element discovery. Rather, they should be weighed on a case-by-case basis. As clause I.7 states:

The TWG has also come to the conclusion that it is not feasible to specify criteria, or combinations of criteria, that, in the words of its Terms of Reference “must be satisfied..” in order to achieve recognition of the existence of a new chemical element and that would cover all cases. Very few properties indeed, of which perhaps the only uncontentious example is the characteristic X-ray spectrum, unambiguously determined, are sufficient of themselves to establish the existence of a new element. For the rest, identification must rely upon combinations of properties that will vary from case to case and that cannot usefully be exhaustively codified as a set of criteria. (Wapstra 1991: 882)

It further states:

To adopt any such codification would be to force research into a strait jacket inimical to the spirit of free enquiry. The TWG has therefore discussed, and here presents, those criteria and properties that have been used in the past and that are seen as being of relevance for the future, and gives some indication of the store that it sets by them, but recognises that their relative importance will vary from case to case depending upon the circumstances in which they are displayed and the manner in which they are combined. (Wapstra 1991: 882)

So, the 1991 report acknowledges that it is not clear which set of criteria should be taken as decisive, nor how to interpret them in a way that matches all instances of element discoveries. Instead, it is

recommended that the criteria are weighed on a case-by-case basis, depending on the element that a research team tries to discover. This mentality is further promoted by the second (and latest report) produced by the JWG which was established in 2017 by IUPAC and IUPAP in order to review the criteria that were set in the 1991 report. In the subsequent report titled 'On the discovery of new elements', the JWG adds further criteria but also- more importantly- describes how the criteria should be interpreted, specifying among other things the limits of their applicability (Hofmann et al. 2018: 1822).

Note that this report was produced in light of the following developments. By the time the 1991 report was published, nine elements were left to be discovered. Out of those, four proved to be particularly difficult: elements with atomic number 113, 115, 117, and 118. These were the last elements to be discovered (thus far) in 2004, 2006 and 2010. All of them are highly unstable, superheavy metals, which exist for milliseconds and were synthesised by bombarding heavy metal targets with ion beams. While scientists purported to have acquired evidence as to their discovery, it was very hard to reach consensus as to the validity of their claims.²²

The difficulty in validating such claims arose in large part due to the following problems. There were substantial experimental challenges and subsequent interpretational problems faced during the synthesis of a new element. These problems arose in part because of the flimsy nature of the elements that scientists attempted to discover, but also because of the technological restrictions and problems they faced.²³ When it came to superheavy elements, scientists could (most of the time) only infer that they had synthesised one. That is, it was (and still is, at least for now) extremely difficult to measure the properties of a discovered element.²⁴ As the JWG puts it:

(..) in general the nature of the experimental data is such that an absolutely secure identification in a first discovery experiment is rarely possible when new regions in the chart of nuclei are explored, as it was the case with the discovery of spherical superheavy nuclei at the end of the 1990s. However, combining the information from various irradiations and measurements, the new elements could be safely and relatively quickly identified. (Hofmann et. al. 2018: 1822)

²² For example, element 118 (i.e. Oganesson) was said to be first identified in 2002 by the Joint Institute for Nuclear Research in Russia (lead by Yuri Oganessian). In 2006, the discovery of Oganesson was confirmed and its discovery was officially admitted in 2015.

²³ For example, one problem with synthesising an element by using some form of cyclotron is that in order to produce superheavy elements, scientists have to hit the target with other superheavy elements which however might burn the target.

²⁴ Only fairly recently, in 2010 and 2012, did researchers manage to directly measure the mass of two heavy elements; namely of nobelium and lawrencium (see Block et. al. 2010; E. Minaya Ramirez et al. 2012 respectively).

Note that a more reliable method employed was to track so-called radioactive decay chains (e.g. Hofmann et. al. 2002). A decay chain is a “series of nuclides in which each member transforms into the next through nuclear decay until a stable nuclide has been formed” (IUPAC 2014: 278). Identifying such chains allowed scientists to infer the discovery of a new element by tracking how they radioactively decay into lighter elements.²⁵

Nevertheless, tracking the decay chain of a superheavy element is not always feasible or successful. In fact, scientists are now acknowledging that one cannot always expect to claim the discovery of a new element by conducting a single experiment. The firm approval of an element discovery may require more than one experiments or measurements. As the JWG puts it:

(...) special consideration is needed when the observations of two or more experiments have to be combined for deducing an unambiguous discovery of a new element. In such cases, discovery profiles need to be established by weighting and combining the observations of the different experiments. (Hofmann et. al. 2018: 1793)

Interestingly, this is another feature that differentiates scientists’ modern conceptualisation of element discovery from the standard one held in the past. Element discovery is no longer associated with a single event; namely a “first discovery experiment” conducted by a single person or research group. It may involve a set of experiments that all together affirm and represent the element’s discovery.²⁶

So, the concept of element discovery has gradually, yet importantly, shifted from how it was conceived by the time of Lavoisier, Mendeleev and up to the beginning of the 20th century. It has become a flexible and fluid concept that is specified through an open set of criteria that are weighed and interpreted on a case-by-case basis. Section 3 examines how these difficulties in discovering new elements has led to another conceptual shift; namely that of the periodic table’s predictive power.

3. The predictive power of the periodic table

²⁵ <https://www.chemistryworld.com/opinion/the-criteria-for-discovering-a-new-element/3010459.article>

²⁶ This is strongly connected to the importance of reproducibility; namely to the ability to conduct multiple times a set of experiments so as to check the validity of the initial experimental results (see for example criterion II.2 of the 1991 report (Wapstra 1991: 882)). Of course, this is something that was always to some extent important in element discovery (as in scientific practice more generally). Nevertheless, element discovery became much more collaborative compared to the past when the epistemic difficulties involved in synthesizing new elements required much more scrutiny of the relevant data.

3.1 From filling gaps to tracking physical boundaries

To this day, the periodic table is considered as the main way by which scientists have successfully predicted the existence of new elements. Its ability to predict new elements has been so great that it has been lauded as one of the most successful predictive tools of science in general. Its apparent success- even by the time of Mendeleev's original version- has drawn the attention of philosophers who have invoked the periodic table as evidence of how important predictions are in science.²⁷ For example, Lipton says:

When Mendeleev produced a theory of the periodic table that accounted for all sixty [really sixty-two] known elements, the scientific community was only mildly impressed. When he went on to use his theory to predict the existence of two unknown elements that were then independently detected, the Royal Society awarded him its Davy Medal . . . Sixty accommodations paled next to two predictions. (1991: 134)

The periodic table's predictive power lies in two features. First, it has been able to predict the existence of unknown chemical elements. Even in its original version, Mendeleev had managed to successfully predict the existence of three elements: germanium, scandium and gallium.²⁸ Secondly, due to the periodic trends tracked through the particular orderings of the elements in the table, the table has managed to successfully predict with fair accuracy the value of those elements' physical and chemical properties.²⁹ It is in virtue of these two features that the table is regarded as being predictively powerful.

However, all the gaps in the periodic table are now filled and the last (seventh) row has been completed with the latest discoveries of elements. If there are no other elements to be found, then perhaps the predictive power of the periodic table- as initially construed- is exhausted. Put differently, the table may have run out of elements to predict.

That there may not be (many) other elements to discover is not an unreasonable hypothesis. Based on nuclear physics, scientists regard as fairly uncontroversial that the periodic table has a limit;

²⁷ This discussion in turn has led to a philosophical debate about whether in theory choice, the prediction of novel facts should be regarded as empirically more important than the accommodation of known facts (see Barnes 2022 for an overview).

²⁸ In fact, this is often invoked as the reason why Mendeleev's proposed classification was eventually chosen over alternative classifications proposed (e.g. Lipton 1991).

²⁹ Of course, there were discrepancies in some predictions and in the case of Mendeleev's original table it has been pointed out that some false predictions were made both with respect to the existence of some elements as well as with respect to their purported properties (e.g. Scerri and Worrall 2001).

namely, that there can only be a finite number of elements that can persistently exist.³⁰ This hypothesis is based on Einstein's relativity theory, according to which there is a point beyond which relativist effects no longer allow for a nuclide to stick together. That point marks the final limit for elements; beyond that, one cannot reasonably regard the sum of protons and neutrons as a persisting entity.

However, while scientists consider it fairly uncontroversial that there is a limit to the number of chemical elements, there is little confidence about where that limit exactly lies. At the moment, there are only conjectures. The TWG report for example, states that it expects nuclides with atomic number up to 190 (Wapstra 1991: 884). Others point out that there is no reliable evidence that elements with atomic number beyond 118 are available, even though there are some models which suggest that elements with atomic number up to 172 could exist (Pyykkö, P. 2011; Nazarewicz 2018). Even Richard Feynman made a guess by claiming that the final element is element 137 (which due to that is called Feynmanium) (Feynman 1998).

In light of this, one could still believe that the table may have some role to play in the prediction of elements, thus retaining its predictive power. However, in practice this does not seem to be the case. The most reliable tool that currently guides scientists in their quest for new elements is the nuclear shell model.³¹ According to this model, nuclei have a shell-structure. As such, they are rendered stable when their shells are full or half-full with a specific number of protons or neutrons. Note that this idea is very similar to how chemical stability is construed for atoms. Atoms have an electronic shell-structure and achieve chemical stability when their shells are filled or half-filled with a specific number of electrons. The nuclear shell model makes a similar hypothesis: when a nuclide has filled its shells with the appropriate number of protons or neutrons (or both), then it becomes stable. The number of protons or neutrons which purportedly results in the formation of a stable nucleus is called a magic number. So far, scientists believe that the following numbers are magic: 2, 8, 20, 28, 50, 82, (114), 126 (138, 152 and 164).³²

³⁰ Of course, what it means to 'persistently exist' is a major issue in metaphysics and it would be extremely interesting to examine how the case of chemical elements can inform such a discussion. Due to the scope of the present article, this is left for another occasion.

³¹ It also explains why specific isotopes of known elements are particularly stable (such as helium, calcium, oxygen and nickel). Prior to this model, scientists developed the liquid drop model which was less optimistic about the existence of stable superheavy elements. The model is now discredited by scientists.

³² Some numbers are in brackets because not all scientific sources mention them.

This model is used to predict which isotopic variants of undiscovered superheavy elements could persist in a relatively stable state.³³ Specifically, it is believed that those isotopes whose number of protons and/or neutrons corresponds to a magic number are stable and thus discoverable. The set of all isotopic variants that hold magic numbers are said to form the so-called 'island of stability'. This island is taken to be found within 'a sea of unstable nuclei', and discovering where that island lies has become the most promising way to discover new elements (Hofmann et. al. 2018: 1780).

In light of this, the burden of predicting what new elements exist is no longer carried by the periodic table but by the theory and models developed in nuclear physics. The nuclear shell model guides scientists as to which precise configuration of protons and neutrons they should try to synthesise. By pointing out which of the possible isotopes of a superheavy element is most stable, scientists have a much clearer idea of which nuclides they should attempt to synthesise (i.e. discover). Note that this is information that the periodic table - by its very structure- cannot offer. The table classifies elements in terms of increasing atomic number, and the different isotopes of a given element are not represented distinctly in the table. Instead, they are all represented by a single position. Given this, one cannot predict through the table which specific isotope (i.e. configuration of protons and neutrons) is sufficiently stable.

Another (separate) reason why the table can no longer contribute to the discovery of elements as before, is because there is some empirical evidence suggesting that heavy elements may not comply to the periodic trends posited by the table. Some heavier elements have been found to exhibit discrepancies with respect to the properties that are expected of them based on their position in the table. For example, element 114 (flerovium) belongs to group 14 and period 7, has a closed-shell configuration and was initially expected to behave like a noble gas. However, recent experiments conducted by a research team at Lawrence Livermore National Laboratory have produced evidence that flerovium's volatility and unreactivity is closer to that of radon (of group 18), whereas other properties are closer to those of mercury (of group 12) (Despotopoulos et al. 2016). This has led the team leader of the laboratory to boldly claim that "(f)lerovium might not belong [where it currently sits in the periodic table], so in other words Mendeleev's table is no longer true".³⁴

This is important because part of the predictive power of the table is taken to be grounded on its ability to predict the chemical and physical properties of new elements. Based on their purported position in the table, the table classifies them into a specific group, family and period, and thus infers (from its membership to each set) the value of its chemical and physical properties. With the discovery and study of heavier elements, there is empirical evidence that the table may no longer

³³ Those isotopic variants whose number of both protons and neutrons are magic (called doubly magic numbers) are predicted to be the most stable.

³⁴ <https://www.chemistryworld.com/news/molecular-cages-could-uncover-element-114s-true-chemical-nature/3008861.article>

serve this predictive function for newly discovered elements, as it did with lighter elements in the past. Admittedly, this is still a conjecture as the empirical evidence is based on experiments that study very few atoms at a time and face significant technological and interpretational difficulties (as mentioned above). Nevertheless, it seems that at least in practice the periodic table no longer exercises the same predictive function it did before.

3.2 Is the predictive power of the table lost?

If the periodic table can no longer be used to discover new elements and predict their properties, does this mean it has lost its predictive power? I believe not. Even if indeed it is the case that the periodic table cannot contribute predictively to the discovery of superheavy elements, this does not imply that it has no other predictive functions. In fact, I claim that to evaluate the table's predictive power solely in terms of its ability to predict new elements, misrepresents and undermines its immense predictive value in chemistry and other fields of study.³⁵ So, if anything, we should shift how the concept of predictive power is construed with respect to the periodic table, incorporating all predictive contributions that the table makes in science. This suggestion is much in the same spirit as that which chemists followed when shifting the meaning of the concept of 'element discovery' in light of the difficulties they faced with discovering heavy elements (see section 2).

Beyond the research into new chemical elements, the periodic table serves crucial predictive functions in other fields and research programs, including of course chemistry and physics, but also fields such as palaeontology, biology, astrochemistry and climate science. For example, the study of the periodic table has helped scientists make predictions about gene sequencing in ancient organisms (e.g. McFarland 2019). Williams (1997) retrodicted how early life on earth evolved based on an analysis of the stability of transition metals. His analysis of the periodic table, combined with research in geology and biology, led to astonishing predictions about how chemical transformations lead to the emergence of life. As McFarland puts it, "(b)y following the chemical rules of how oxygen would react and how metals combine and dissolve, Williams argued that life on the ancient earth could only use elements on the left side of the series (manganese, iron, cobalt, and nickel) while more recent, complex life use more elements on the right side of the series (copper and zinc)" (2019; also 2016).

Interestingly, Williams' work also led to predictions about how life could evolve in other water-based planets. In general, there is now significant work done in predicting the chemical constitution of other planets, and of predicting how certain atmospheres may chemically (and potentially biologically) evolve. For example, Doerksen and Fortenberry compared hydrogen-rich environments with environments where hydrogen decreases and claim that the former "may very

³⁵ It is on this basis that I have argued elsewhere that the periodic table identifies many laws of nature (e.g. Seifert (accepted/in press).

well favour gas phase formation of small molecules containing inorganic and refractory atoms” (2021: 4). This claim was based in part on analysing the ability of different elements of the periodic table to form single, double and triple bonds and evaluating which elements (from those that are more abundant in the atmosphere of Earth and of other planets) could form the strongest bonds (and with which elements).

All in all, philosophers and chemists have conceived the table’s predictive power primarily in terms of its ability to predict new elements. However, this misrepresents the actual value of the table. The periodic table serves an important predictive function in chemistry more broadly, but also in other fields of study such as astrochemistry and biology. To diminish the predictive power of the periodic table on the grounds that it no longer contributes to the discovery of new elements would misrepresent the actual predictive role the periodic table holds in science today.

4. Conclusion

I argue that recent developments in the discovery of elements suggest the need for a shift in how we construe the concepts of element discovery and the periodic table’s predictive power. In the case of element discovery, such a shift has already occurred in chemical practice and explicitly acknowledged by the relevant scientific institutions which now propose a much more flexible understanding of this concept.

With respect to the periodic table, I point out that its predictive power no longer lies in its ability to successfully predict elements and their position in the table. This reflects a significant conceptual shift because the periodic table has been one of the most celebrated case studies of successful predictive tools in science on the basis of its predictions of new elements. However, I claim that we need not accept that the periodic table has lost its predictive power. The role of the table in chemistry, as well as in physics, biology, astrochemistry and other fields of study, shows that it still plays a very important predictive role. So, if anything, this is evidence that - just as with the case of ‘element discovery’ - we should change how we construe ‘predictive power’ when it comes to the periodic table.

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