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Causation, electronic configurations and the periodic table

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Abstract

The article examines a recent interventionist account of causation by Ross, in which electronic configurations of atoms are considered to be the cause of chemical behavior. More specifically I respond to the claim that a change in electronic configuration of an atom, such as occurs in the artificial synthesis of elements, causes a change in the behavior of the atom in question. I argue that chemical behavior is governed as much by the nuclear charge of an atom as it is by its electronic structure. It is suggested that an adequate analysis requires attention to the dynamical interactions between nuclear charges and those of electrons, as typically carried out through the application of the Schrödinger equation. It is concluded that electronic configurations can only be said be causal in a weak sense that is somewhat analogous to the causal arguments that are invoked in folk physics.

Keywords Causation · Electronic configurations · Periodic table · Chemistry · Quantum chemistry

1 Introduction

The following article is concerned with causation in relation to electronic configurations of atoms and the periodic table of the chemical elements. Some of these issues were recently discussed in this journal by Ross (2018). In this article Ross suggests that electronic configurations of atoms play a causal role in determining the properties of the elements and claims that the periodic table provides explanations in chemistry.

Ross points out that many chemists seem to regard the periodic table as providing genuine explanations for chemical phenomena. However, she appears troubled by the fact that some philosophers of chemistry have taken a more critical view over the question of whether there is a causal relationship between the electronic structure

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of atoms and their chemical behavior (Scerri 1997; Woody 2014). Ross wishes to argue that the periodic table does indeed provide causal explanations for the chemical behavior of any particular element and more specifically that the causal explanation does indeed lie at the level of the electronic configuration of the atoms of any particular element.

The present article is intended as a further examination of these issues. My overall message will be that although Ross may be correct in attributing some causal and explanatory role to the periodic table and also to the electronic configurations of atoms, such a role lacks depth. Instead I argue that an appeal to the Schrödinger equation for the system, or the chemical reaction in question, provides a deeper set of explanations and even a causal role if one insists on speaking in such terms.

In presenting her case Ross follows the interventionist account of causation which has been presented by James Woodward (2003). According to this account causal relationships take place among variables which represent properties capable of taking on differing values. Woodward holds that to say that X is a cause of Y means that changes in X produce changes in Y in some background circumstance. Consider the well-known example, that of a light switch that can take on either of two possible values of on or off. Similarly, a light bulb to which the switch is connected can also take on two values, namely on or off. The fact that changing the state of the light switch results in a change in the light bulb, from showing no light to being on, is taken to mean that the operation of the switch is a cause of the bulb's alternative states.

Needless to say, Woodward and Ross are well aware of the fact that there may be occasions in which the light switch may be manipulated correctly but the light may still not come on, perhaps due to a malfunction in the switch or the light bulb filament or perhaps both. Nevertheless, these authors still wish to consider the switch to be the cause of the state of the light bulb, and not unreasonably so. The deeper cause of the light bulb's state is of course the detailed physics of how operating a well-functioning switch results in the flow of a current through a suitable conductor and the accompanying physics that takes place to convert an electric current into a glowing metal filament within an evacuated tube.

2 The interventionist account applied to the periodic table

The novelty in Ross' article lies in applying Woodward's account to the periodic table of the elements and extending the light bulb example to cases in which many different states can be adopted by the putative cause as well as the putative effect. In the case of properties of elements, for example, the possibilities are in principle limitless rather than the simple on/off displayed in the case of the light bulb.

Ross makes the following claim for what she terms a "figure", such as the periodic table, if it is to be considered as being causal according to the interventionist account.

> These considerations suggest three criteria that a scientific figure should meet if it contains causal structure or causal information. At the very least, such figures should specify (i) some cause variable C that can take on different values, (ii) an effect variable E that can take on different values, and (iii) how values of

> C systematically relate to values of E in the interventionist sense (I) captured above (Ross, 2018, p. 5).

Ross also raises the question of what this account of causation has to do with explanation. Her response is that causal explanations are often characterized as the explanation of some effect by appealing to its causes, and that on the interventionist account an explanandum is represented by some range of values in an effect variable. Meanwhile the corresponding explanans involves some cause variables and how its different values systematically relate—in an interventionist sense—to the range of values in the effect. According to Ross, the hallmark of causal explanation involves supplying the relevant difference making information in the causes, something that is not found in other scientific activities such as classification, prediction or description of phenomena.

Ross then turns to the familiar vertical groups and horizontal periods in the standard periodic table of the elements. She considers the property of atomic radius and how it increases as one moves vertically down any group or column, whereas it decreases on moving horizontally from left to right along any given period. These trends are regularly invoked in chemistry in the course of qualitative discussions about how properties vary among the elements. But as Ross correctly emphasizes, chemists are also interested in explaining properties in addition to describing them in qualitative terms. The explanations are provided from the more theoretical parts of chemistry, which Ross identifies with the electronic structure of the elements. Before moving on, let me mention that I believe that Ross takes the latter notion a little too literally to mean the electronic configurations of atoms of the elements, or a count of the number of valence, or outer-shell, electrons possessed by any particular atom. In fundamental terms "electronic structure" is regarded more broadly than just a stipulation of the number of valence electrons, in a way that Ross does not consider and that I will explain below (Scerri 2020).

Ross also provides various quotations from general chemistry textbooks to illustrate the point that chemical explanations are generally afforded by referring to the electronic structure of the atoms of the elements in question. I believe that restricting oneself to general level undergraduate textbooks can serve to confuse the situation, as I will attempt to explain.

Returning to cause and effect, Ross identifies the properties of elements as the explananda or effects. She draws on the interventionist account of causation to say that a particular group or periodic trend can be represented by a variable P that is capable of taking a range of values and that the different values it can adopt are specified by changes as one moves through the periodic table.

According to Ross the explanans are provided by the electronic configurations of the atoms of any particular element. As she correctly points out, chemistry textbooks regularly invoke the electronic configurations of atoms as a way to explain chemical behavior.

> I am going to suggest that the way to understand these claims–and the main feature of these explanations–is that electronic structure and to a significant extent atomic structure, are causally responsible for various chemical and physical properties of the elements in an interventionist manner. These atomic features

> “make a difference” to these properties in the sense that changes in these features produce changes in these properties (Ross, 2018, p. 18).

She also writes,

> As chemists state, “periodicity is a consequence of the variation in ground state electronic configurations” and “[e]lectron configurations of elements help to explain the recurrence of physical and chemical properties” (Housecroft and Sharpe 2010, p. 20; Chang 2007, p. 326). Thus, serially ordered elements exhibit periodic changes in their properties, because these properties are caused by atomic features which themselves vary periodically with this ordering. This involves explaining repeating changes in an effect by appealing to repeating changes in its causal factors (Ross, 2018, p. 12).

> What exactly does it mean to say that these atomic features explain these properties? Some of these explanations have a causal interpretation and are well understood within an interventionist framework. In these cases, chemists are stating that these atomic features are causally responsible for these chemical and physical properties in the sense that if one were to intervene on and manipulate these features this would produce changes in these properties and, relatedly, variations in these properties depend on variations in these features (Ross, 2018, p. 12).

In order to further bolster this proposal that a change in electronic structure brings about a change in chemical behavior of an element, Ross appeals to theories of the Big Bang creation of the universe and current ideas on the artificial synthesis experiments that have produced as many as 26 new elements beyond the element uranium in the periodic table. As Ross notes, the artificial synthesis of elements began when Rutherford and Soddy succeeded in converting an isotope of nitrogen into one of oxygen by means of alpha particle bombardment. Ross takes such experiments as a vindication of the notion that a change in electronic structure results in changes in chemical and physical behavior.

Let me pause to raise a minor objection to this claim, since what is really being changed in any of the above-mentioned examples is not electronic structure but in fact nuclear structure. When Rutherford and colleagues were able to convert nitrogen into oxygen, what they achieved is represented in the following chemical equation,

$$ {}^{14}_{7}N + {}^{4}_{2}He \rightarrow {}^{17}_{8}O + {}^{1}_{1}H $$

Stated in words this equation signifies the conversion of a nucleus containing 7 protons and 7 neutrons into one containing 8 protons and 9 neutrons (Rutherford 1919). Strictly speaking this has nothing to do with electronic structure. In order to make the connection that Ross does, one has to assume that the oxygen atoms that are formed would each have captured an additional electron, something that may or may not occur in general.[1] The fact remains that this is not a case of a direct manipulation of electronic structure that is followed by a change in chemical behavior of the resulting neutral atom.

3 Some further concerns

I believe that there may be a more serious problem with Ross' account in that it would seem to apply only to some properties. Had Rutherford obtained ^{17}O in a sufficient amount rather than the far more common isotope of ^{16}O, it would presumably have behaved like oxygen in terms of its chemical reactivity. However, some of the properties of isotopes of any particular element, and especially their compounds, vary considerably. Consider for example water or H_2O and heavy water, or D_2O, where D denotes atoms of deuterium or ^2H. The freezing point of D_2O is about 4 °C, compared with 0 °C for H_2O while the temperatures of maximum density are 11.6 °C and 3.9 °C respectively. Even more dramatically, ingesting H_2O is essential for life whereas the ingestion of even a small quantity of D_2O can cause death in fish.

The bond vibrational frequencies of molecules are also highly isotope dependent. To return to Rutherford's ^{17}O, one can easily compare the vibrational frequencies of the ^{12}C–^{16}O and the ^{12}C–^{17}O stretching modes in the carbon monoxide molecule for example. If the frequency of one of these vibrational modes is known it is an easy exercise in undergraduate chemistry to calculate the frequency of the other one by using a classical approximation.[2] For the carbon monoxide molecule the heavier molecule, consisting of ^{12}C–^{17}O, has a vibrational frequency that is lower than that of ^{12}C–^{16}O by approximately 27 cm^{-1}.

Certainly the manipulation of an atom of nitrogen results in the formation of an atom of oxygen, that has the typical reactions of oxygen. However, as I have argued, it does not yield an atom with all the properties that would correspond to a natural sample of the element with a particular abundance of isotopic masses. This is why I believe that equating the manipulation of nuclear structure with the implied manipulation of electronic structure, that is supposed to follow, is not as straightforward as Ross would have us believe.

The periodic table is mainly concerned with electronic structure and not nuclear structure. If we are to accept the view of causation in terms of making a change in an atom, it should be a change that produces a typical atom of the new element and not just one particular isotope. The production of a range of isotopes of one particular element

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[1] This is an issue in the field which attempts to synthesize super-heavy elements. It is usually taken that the time required for a nucleus to capture electrons is 10^{-14} s. Any nucleus whose half-life is shorter than this period does not even count as a genuine element (Kragh 2018).

[2] This kind of calculation is regularly carried out by first year undergraduate students in a general chemistry course at a major institution such as UCLA where I teach such courses. The calculation involves using the expression for the vibrational frequency of a classical vibrating spring, namely $v = 1/2\pi\left(\frac{k}{\mu}\right)^{1/2}$ where k is a force constant characterizing the stiffness of a spring, or of a chemical bond, and μ is the reduced mass of a system consisting of two masses m_1 and m_2, where $\mu = m_1 \cdot m_2/(m_1 + m_2)$. Given that the approximate frequency for ^{12}C–^{16}O stretching mode is 2143 cm^{-1}, that of ^{17}O–H is calculated to be approximately 2116 cm^{-1}.

is not what takes place in practice however, given that the experiments in question involve the collision of a particular isotope of an element with an α particle or with any particular isotope of another element. Nucleosynthesis, of the form conducted artificially on earth, is isotope specific, while Ross' argument ignores any differences between the isotopes of any element, either the target atom or the isotope produced.

Although the periodic table was discovered by chemists like Mendeleev, chemists do not hold a monopoly over the periodic table. In discussing the properties of atoms and elements we are equally entitled to discuss their more physical properties as we are their chemical properties. The manipulation of ^{14}N to form ^{17}O can indeed be physically achieved, as it first was by Rutherford, but this is not the same as changing a nitrogen atom featured on the periodic table into an oxygen atom that also appears on the periodic table.[3] Ross appears to conclude that the two conversions are equally feasible.

Although this distinction does not matter for chemical properties, it does when it comes to in general properties.[4] So although Ross' argument seems appropriate in a general sense, there is a sizeable gap to be bridged before we might become capable of manipulating atoms in order to produce other atoms that take up a different position in the periodic table.[5]

4 Towards a deeper account of causal explanation

Ross claims that if one changes the electronic structure of an atom, or more specifically the structure or configuration of its outer shell electrons, then one produces a different electronic structure that can be identified with causing the properties of the newly formed atom. I have already pointed out that such manipulation takes place directly in the nucleus rather than in the electrons. I have also pointed out that a consequence of this fact is that we must speak of isotopes of the target, as well as the product atom, and that one thereby loses the specific one-to-one relationship, which Ross is claiming on moving from nitrogen to oxygen à la Rutherford.

But there is yet another problem lurking behind the scenes, which can be illustrated by considering the change from a nitrogen atom to one of oxygen, as well as the analogous change from an atom of phosphorus to one of sulfur.[6] In terms of outer-

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[3] The periodic table features idealized or average atoms, each of their weights being taken over all the isotopes of that element, except in the case of monoisotopic elements.

[4] I am not however implying that there exists a clear-cut distinction between chemical and physical properties.

[5] Stated more precisely, most of the atoms that are represented on the periodic table do not actually occur in nature. These "average atoms", as I have called them, are the result of taking a weighted average of the masses of all the isotopes of a particular element. For example the periodic table shows that an atom of hydrogen has a mass of 1.008 atomic mass units. But in reality there is no such atom since this value is arrived at by taking the weighted average of the masses of the three isotopes of hydrogen or approximately 1, 2 and 3 atomic mass units respectively for ^{1}H, ^{2}H and ^{3}H. The only elements for which the atomic mass shown on a periodic table corresponds to an atom that actually exists are the 20 or so mono-isotopic elements such as Be, F, Na, Al, P, Sc, Mn, Co, As, Y, Nb, Rh, I, Cs, Pr, Tb, Ho, Tm, and Au.

[6] Phosphorus lies directly below nitrogen in the periodic table, while sulfur lies directly below oxygen. This reflects the fact that each of these pairs of elements share numerous properties.

shell configurations both manipulations would involve a change from a configuration of ns^2p^3 into one of ns^2p^4. In other words the change achieved via the manipulation would result in a change from 5 to 6 valence electrons. How could such a mere numerical change capture the difference in the properties of each of these pairs of elements which are vastly different? Moreover, if numbers of electrons were the only factor, it would imply that all the elements in each group should behave in an identical manner, something that clearly contradicts the facts.

Although the periodic table embodies the notion that elements repeat themselves, as it were, after certain regular intervals, this is accompanied with the knowledge that such repetitions are approximate. Restricting the characterization of atoms to just their outer-shells severely under-determines the chemical and physical behavior of atoms.

The notion of electronic configuration per se does not therefore stand up to close scrutiny as anything but a simplified example of causation, not altogether unlike the earlier discussed case of the switch and light-bulb. Nevertheless, to be fair to Ross, causal explanations within interventionism are just descriptions of how an effect would change if a cause were changed, but this is also why such a causal account lacks depth in the view of the present author.

5 The role of quantum mechanics

What causes the properties of any particular atom is the complex dynamics that exists between a particular number of electrons and the nucleus in question.

Consider for example the difference between an atom of hydrogen and one of helium. In the case of hydrogen there is just one contributing potential energy term, that of an attraction between the nucleus and the electron, namely $-e^2/r$ where e represents the charge on the electron and r the distance between the nucleus and the orbiting electron.[7] In the case of the helium atom there are two electrons and as a result there are two terms to the one that is present in hydrogen.[8] But in addition there is an all-important electron–electron repulsion term given by $+e^2/r_{12}$.

$$\text{Hydrogen: Potential Energy} = -e^2/r$$

$$\text{Helium: Potential Energy} = -2e^2/r_1 - 2e^2/r_2 + e^2/r_{12}$$

To consider the change from the hydrogen atom to that of helium to be due to a change from one to two electrons, or from configuration $1s^1$ to $1s^2$, is to fail to include the electron–electron repulsion term. Chemistry is not just about a particular number of electrons but about the forces within any particular atom which, as can be seen, do not correlate precisely with the mere number of electrons.

Expressed in different terms, the use of electronic configurations as a causal or explanatory device is an over-simplification of the facts. A deeper explanation lies

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[7] The electron has a charge of $-e$ while the nucleus of hydrogen has a charge of $+e$. The product of the two charges gives $-e^2$, where the resulting negative charge denotes an attraction between the two particles.

[8] Another difference is the nuclear charge on the helium nucleus which is $+2e$.

in the force dynamics, which are captured in the Schrödinger equation of the atom in question.[9] Moreover, any differences between the atoms of any two elements are due as much to the different nuclear charges as they are to the number of electrons. Meanwhile, an electronic configuration does not contain any information about the nuclear charge of an atom.

This is why rigorous explanations in chemistry and physics currently require quantum mechanics. It is also why generally speaking professional chemists believe that quantum mechanics provides genuine chemical explanations while electronic configurations are a useful but crude generalization. Electronic configurations of atoms, and of molecules too, are more useful in chemical education than in 'real-life chemistry'. When a chemist wishes to predict the behavior of an element or a compound, or the bond angles within a molecule, or indeed any number of properties she reaches for her quantum mechanical computer program. Meanwhile, knowing the electronic configuration of the atom or molecule is of rather limited use, apart from making qualitative comparisons with other elements (Scerri 2020).

6 Explanation, classification and causal structure

In the fourth section of her article Ross turns to examining explanations in chemistry and the kinds of explanations that are afforded by the periodic table. She readily acknowledges that the table "doesn't explain everything about elemental properties" but maintains that the periodic table provides "at least some causal structure". My own purpose in the resent article is to examine the depth and extent to which the periodic table provides such causal structure.

> This isn't to say that the table explains everything about elemental properties that one might be interested in or that it contains maximal atomic detail about such explanations. Surely there are explananda that the table doesn't address and it clearly omits details that may provide "deeper" or more "complete" understandings of those phenomena it does. A main goal of this paper is to show how this table contains at least some causal structure and, thus, that figures in at least some explanations without suggesting that these are the only explanations of periodicity in this domain or even that they are as detailed as (other) explanations that invoke more atomic theory (Ross, 2018, p. 15).

Ross then mentions the fact that these features, namely the failure to fully explain elemental properties, including the occurrence of periodicity itself, have been taken by some philosophers of chemistry, including myself, to mean that the table is not explanatory. This is a view that Ross rejects since as we have seen she considers that the identification of causal connections through electronic configurations, on her interventionist account, shows that the periodic table per se does in fact provide explanations.

My objection to the table having explanatory value per se is that the periodic table is only a chart or a graphical classification rather than any form of deep explanation.

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[9] In addition there are quantum mechanical exchange terms that have no classical analogues.

Needless to say, I have no objection to the notion that the periodic table interpreted through the electronic configurations of its atoms can provide at least *some* causal structure and can therefore serve at least some explanatory role.

More specifically Ross refers to articles which point out that whereas ab initio quantum mechanics gives a prediction of the number of electrons that may fully occupy and electron shell, namely 2, 8, 18, 32, 50 etc., the same theoretical account does not predict the elements at which chemical periodicity occurs. To explain further, if one adds the numbers of electrons in each shell, as shown above, one would predict that the closed shell atoms, or noble gases, might occur at the cumulative totals of 2, 10, 28, 60, 110 electrons, whereas the nobles gas atoms have 2, 10, 18, 36, 54, 86 and 118 electrons. Ross writes,

> This criticism appears to be guided by an expectation that proper explanations should be "complete" in some sense and should involve derivation from lower-level theories, similar to a deductive nomological (DN) approach (Ross, 2018, p. 15).

I would like to explain why this appearance, as Ross calls it, is mistaken. It would of course be very naïve to believe that one can ever hope for a complete explanation. I certainly do not subscribe to such a view. However I do believe that an over-riding goal in all of science is to seek ever deeper and more encompassing explanations for any phenomenon. Such a goal does not owe any allegiance to a particular philosophical doctrine such as the deductive nomological approach as Ross suggests that I believe. It is merely the motivation that has driven all of science from the beginning, namely to seek ever deeper explanations, preferably explanations that can be deduced from theories without importing any information that one is attempting to explain. Stated in other words, I believe the more ab initio and the less semi-empirical explanation might be, the better the explanation. This motivation did not need to wait for the advent of logical positivism and the D-N approach to scientific explanation. It is rather a commonplace view, among physical scientists in particular.

Meanwhile, Ross believes that the approach that I support,

> …places an unrealistically high bar on what on what counts as explanatory, in the sense of assuming that explanations should be "rigorous" or "complete" with respect to the number of phenomena that are addressed. Where chemists appeal to the order of electron filling to explain patterns in elemental properties, these criticisms suggest that if a genuine explanation goes deeper–it should also explain why electrons fill in this order. One clear worry with this approach is that it can lead to an infinite regress in the phenomena to be explained. (Ross, 2018, p. 15).

I believe that this claim only serves to confuse the issue. It is important to separate clearly two aims of theoretical chemistry in this domain. First of all theorists may attempt to predict, or explain after the facts in some cases, the properties of a particular element's atoms. Secondly, they may also attempt to predict the order of orbital filling of electrons from first principles as one moves through the periodic table. This second activity is more relevant to chemical periodicity since it leads to an understanding of why certain elements have analogous electronic configurations. It is claimed by some authors that this order of orbital filling has been predicted from first principles (Allen and Knight 2000; Belokokos 2017; Bent and Weinhold 2001; Ostrovsky 2001; Kholodenko 2019), although others have disputed the claim (Scerri 2019).

But when it comes to discussing causation in the context of the periodic table, or the project that Ross is mainly engaged in, it is the first of these projects that is more relevant. My claim is that causation is occurring at the level of the quantum mechanical dynamics of atoms rather than at the level of their electronic configurations. One does not need to know the order of orbital filling if one wants to calculate the properties of say an atom of oxygen. One needs to solve the Schrödinger equation for this system consisting of a nucleus containing eight protons and eight orbiting electrons. In fact high-level quantum mechanical calculations do not make any reference whatsoever to the configuration of the atom.[10]

The question of whether the order of orbital filling has been derived from first principles is therefore something of a distraction that I suggest should be kept out of the discussion of what causes operate in the context of the periodic table.

7 Conclusion

To conclude, we should perhaps consider the role of causation in science in general. As is well known, the D-N account of scientific explanation came under intense criticism when a number of counter-examples emerged, such as the case of the flagpole. Whereas the height of the flagpole can serve as an explanation for the length of the shadow that it forms, the reverse is not true. There is no sense in which the length of the shadow can be said to be said to explain the height of the flagpole. Because of examples of this kind, it became generally accepted in the philosophy of science that causes needed to be included in scientific explanations (Salmon 1989). The inclusion of causes then allows us to say that the flagpole causes the shadow but not vice versa.

More recently there appears to be a return, at least in the philosophy of physics community, to the denial of any fundamental role that causes might play in scientific explanations. For example, as John Norton writes,

> I urge that the concepts of cause and effect are not the fundamental concepts of our science and that science is not governed by a law or principle of causality (Norton, 2003, p. 1).
>
> Mature sciences, I maintain, are adequate to account for their realms without need of supplement by causal notions and principles. The latter belong to earlier efforts to understand our natural world, or to simplified reformulations of our mature theories, intended to trade precision for intelligibility. In this sense I will characterize causal notions as belonging to a kind of folk science, a crude and poorly grounded imitation of more developed sciences (Norton, 2003, p. 2).

As many authors have suggested, the need to invoke causes appears to depend on the branch of science concerned (Lange 2013). The more fundamental the science the

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[10] This is especially true of the most common quantum mechanical approach used these days, namely density functional theory.

less that need exists, with physics as the most fundamental science, closely followed by chemistry.

The focus of the present article has been the periodic table and the intersection of chemistry and physics. The explanations for the periodic table and the properties of atoms of the elements is essentially mathematical and to a first approximation is provided by the Schrödinger equation.[11] Causes are not invoked in such explanations but that is not to say that invoking electronic configurations as causes, as Ross does, or as sometimes found in chemistry textbooks is futile. Perhaps we should consider these causal explanations in the same general way that Norton has described the explanations found in folk physics in the above cited passage.

The causes that are invoked by appeal to the periodic table lack depth because they involve qualitative arguments. In addition, the kinds of causes that are directly obtained from the periodic table per se lack specificity. For example, one could argue that an element in group 14 of the periodic table typically forms four chemical bonds and that this is caused by their atoms having four outer electrons. However, such reasoning applies to at least five elements, namely carbon, silicon, germanium, tin and lead.[12] Consequently any appeal to the four electrons as causing chemical bonding lacks specificity.

By contrast, quantum mechanical calculations can be carried out on specific elements and their compounds in order to predict or explain many specific properties that these elements and their compounds might have to a high degree of accuracy. Quantum mechanical calculations can therefore point to deeper causes, even if they cannot be visualized as easily as a particular number of outer electrons can be.

I conclude that electronic configurations do not play anything more than a simplified causal role but that they only serve as such in a sense approaching folk chemistry, to coin a term by analogy to folk physics that philosophers sometimes refer to.[13] Similarly, I do not believe that the periodic table provides genuine scientific explanations even though it may appear to do so in the simplified accounts of chemistry as expressed in elementary textbooks.

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[11] More accurate calculations require the inclusion of relativistic effects (Pyykkö 2011).

[12] It should be noted that tin and lead have a tendency to form two rather than four bonds as a result of the inert pair effect.

[13] Throughout this article I have discussed the term electronic configuration as though the term was unambiguous. I note that some authors believe that more relevant explanations of chemical facts require the use of configurations of bonded atoms of the elements rather than those of gas phase atoms that are usually discussed in chemical education. Moreover, calculations invariably utilize a combination of many electronic configurations of atoms in addition to the so-called ground state configuration (Jensen 2007; Granovsky 2011). Finally, although I have concentrated on the Schrödinger equation approach to computational chemistry in this article, the related approach known as density functional theory has also contributed to the great increase in accuracy of chemical calculations over the past 30–40 years (Burke et al. 2005; Koch and Holthausen 2002). Needless to say, the density functional approach also seeks to capture the detailed dynamical interaction between nuclei and electrons in the system in question rather than to just focusing on the system's electrons.

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