

Chapter 4

A Novel Approach to Emergence in Chemistry

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4.1 Introduction

As noted by Kim (2006), “emergence” is a philosophical term of art. There is no unique or unified theory of emergence, and the meaning of the term varies from author to author. Many scientists with a philosophical bent love the term, as do some philosophers. But others complain that “emergence” is too vague and unhelpful. Despite this, there is a common set of features that many concepts of emergence share. Philosophers and scientists use the term “emergence” in relation to levels of reality. The picture often invoked is that of a layer cake: physics at the bottom, followed by chemistry, biology, psychology, etc., where each level is seen as harbouring novel entities,¹ properties, phenomena, which emerge from the interactions at the lower level.² This picture may be problematic, but if one accepts it, emergence is seen like a nice way to explain the relations between the levels.

When thinking about emergence in this way, two seemingly contradictory features become apparent. On the one hand, the emergents (be they entities, properties, phenomena, processes, laws, explanations, etc.) are seen as *dependent* on the lower level; on the other hand, emergents are seen as being *autonomous* from the lower level. These two features seem contradictory: how can one and the same set of things, properties, etc. be at the same time dependent and autonomous from another set of things, properties, etc.? I suspect this is one of the reasons

¹ Throughout this paper I am using the word “entity” to mean “concrete individual” or “object”.

² The metaphor of the layer cake is due to Putnam and Oppenheim (1958), who adopted it to argue for a certain kind of reductionism.

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why emergence is sometimes seen as an incoherent position. But perhaps it need not be; perhaps there is a sense in which dependence and autonomy can coexist. A challenge that emergentists face, therefore, is to explain precisely how this can be. One way to do this is to conceive of dependence in terms of supervenience, and of autonomy in terms of the failure of reduction.³ Thus, emergence can be seen as a version of nonreductive physicalism: *physicalism* because virtually all approaches to emergence recognize that at the basis, all there is is physical – the higher strata are seen as supervening on the physical; *nonreductive* because, for one reason or another, the higher levels do not reduce to the lower level.

Some authors go beyond this picture and see emergence as depending on downward causation (Hendry 2006). Others do not consider downward causation as a necessary condition for emergence (Batterman 2002). In this paper I will assume a fairly liberal concept of emergence – arguably, a theory which does not include downward causation can still be a theory of emergence if it talks about levels of reality which are dependent but autonomous from one another.

Developing theories of emergence can be useful to those who are concerned with the disciplinary autonomy of the special sciences. Since the emergents at one level are autonomous in relation to the lower level, it is natural to think that the science studying them is autonomous from the science studying the lower level. The autonomy of chemistry from physics continues to be debated. Some authors have attempted to ground the autonomy of chemistry in a philosophical position called internal realism (Lombardi and Labarca 2005). But others have argued that chemistry cannot be autonomous from physics if it reduces to it (Manafu 2013b). Thus, insofar as some kind of failure of reduction seems to be a central ingredient of emergence, emergence could perhaps account for the autonomy of chemistry.

Of course, whether chemistry is autonomous from physics depends on how one conceives of autonomy. Unfortunately, the notion of disciplinary autonomy has not been analyzed sufficiently in the philosophy of science. Many philosophers of science rely on an intuitive and implicit notion of autonomy.⁴ One can distinguish between several types of autonomy. First, one can talk about historical autonomy. Historically, chemistry has been independent from physics. It has been claimed that chemistry had become a science “of great extent and certainty” long before we had any mechanistic insight into the internal make-up of the elements (Broad 1925). Broad argued that for a long time, progress in chemistry was possible without using

³ A set of properties H supervenes on a set of properties L if and only if (i) any two objects x and y that have the same L properties will necessarily have the same H properties (though not necessarily viceversa), and (ii) any two objects z and w that differ in their H properties will also differ in their L properties (though not necessarily viceversa).

⁴ Hendry (2012) is an exception, but he does not give many details. He writes: “A science is autonomous if its laws and explanations make no appeal to the laws or categories of other sciences.” (Hendry 2012, p. 382).

any mechanistic assumptions. He concluded that the possibility of mechanistic explanation is not essential to the progress of chemistry.

If then chemistry can be a scientific subject and can make steady progress without using the assumption that a mechanistic explanation of chemical phenomena is possible, it would presumably have made precisely the same progress if in fact no such explanation had been possible. (Broad 1925, p. 74)

While Broad is correct to point out that progress in chemistry happened long before modern mechanistic explanations of chemical phenomena became available, it is also true that the mechanistic insights that became available in the twentieth century have allowed for a great expansion of our chemical knowledge. They allowed us to better understand the chemical reactions that we knew about, and to design new reactions. They allowed us to synthesize new molecules, and even new elements, and to design and create new drugs and materials. In other words, chemistry would not have made precisely the same progress if quantum mechanics had not been discovered, although for a long time its own progress was independent from the progress of physics. Therefore, the autonomy of chemistry in relation to physics cannot be based solely on the notion of historical autonomy, which is also only partially defensible.

A second type of autonomy is methodological autonomy. In general, a chemistry lab looks very different from a physics lab and what goes on in a chemistry lab is different from what goes on in a physics lab. But one may respond to this by saying that while physics and chemistry differ with regard to their methodologies in general, the methods of some branches of chemistry are in fact physical in nature. For example, the bond length and angles of molecules are determined using various types of spectroscopy. Spectroscopy is used in physical and analytical chemistry to identify the composition of substances or to assess the concentration of a given chemical species; computational methods that make use of quantum mechanics are used to determine the structure of compounds. Although in general the methods of chemistry and physics are quite different, this does not demonstrate that chemistry is autonomous from physics. This is because the entities and properties that form the subject matter of chemistry could still be physical entities or properties, even if they are studied with non-physical (i.e., chemical) methods. Thus, what philosophers have in mind when they talk about the autonomy of chemistry in relation to physics is not captured solely by historical or methodological autonomy.

A stronger notion of autonomy can be discussed – the so-called *ontological* autonomy of chemistry. Indeed, this stronger notion of autonomy is the one which presents the most philosophical interest. But what does it amount to? I make the following proposal: a discipline is ontologically autonomous from another if the ontology of the first is distinct from the ontology of the second. To be informative, this proposal must specify what it is meant by “ontology”. Luckily, we have a pretty decent understanding of what an ontology is. Arguably, an ontology must

include: entities, processes, phenomena, properties, laws. To this list one may add explanations, if they are viewed ontically, not just epistemically.⁵ If all these turn out to be physical entities, properties, etc. in disguise, then it is pretty clear that chemistry cannot be autonomous from physics. For chemistry to be ontologically autonomous from physics, chemistry must talk about its own entities, processes, properties, laws. These must be *sui generis*. In other words, they must be *chemical* properties, laws, etc. in their own right, not just species of physical properties, laws, etc.

The ontological autonomy of chemistry is tied with the failure of (at least some versions of) reductionism. Indeed, if all chemical laws are obtainable from quantum-mechanical laws, then how could the belief in the autonomy of this discipline be maintained? Since emergence makes possible the existence of *sui generis* chemical properties, laws, and explanations, it is natural to think that emergence can justify the ontological autonomy of chemistry.

Here is the plan of this paper. The next section summarizes the current state of the debate regarding ontological emergence in chemistry. The current approaches to ontological emergence in chemistry have been met with scepticism, and some have argued that the appropriate attitude regarding ontological emergence in chemistry is agnosticism (Scerri 2012). In the third section I offer a novel approach to emergence in chemistry; the approach is in some sense weaker than the existing approaches, but I argue that it can justify the ontological autonomy of chemistry. In the fourth section I discuss a couple of objections to this approach and speculate a bit on what it entails about the nature of chemistry as a science and about the appropriate model of the relationship between the special sciences. The concluding section summarizes the main points.

4.2 The Present State of the Debate About Emergence in Chemistry

There are several contemporary approaches to emergence which are applicable to chemistry, including Humphreys (1996, 1997a, b), Luisi (2002), Hendry (2003, 2006, 2010a, b), Llored (2012).⁶ In this section I will focus only on some accounts which claim to be ontological (as opposed to merely epistemic) and which apply explicitly to chemistry. More precisely, I will be focusing on the account of emergence recently defended by Hendry.

⁵ An ontology includes objects, phenomena, as well as relations between them. If one includes explanations, then they could be regarded as objective relations between laws and phenomena. The idea that explanations could be seen ontically does not sound as implausible if one thinks that it makes sense to say that for a certain phenomenon an explanation exists but it may never be found.

⁶ For a comprehensive review see Manafu (2013a).

To understand the present state of the debate it is useful to start with Broad, for whom chemistry “seems to offer the most plausible example of emergent behaviour” (Broad 1925, p. 65). It is useful to do so because Hendry’s account is relying on Broad’s. Broad uses an older distinction made by Mill (1882) between purely mechanical behaviour and chemical behaviour. For Broad, a system is emergent if its properties cannot be predicted from a knowledge of the properties of its constituents taken separately or in other wholes, including knowledge of their inter-relations. According to Broad, the only way to learn about the chemical properties of a chemical compound is empirically, by studying samples of that compound. If we start with knowledge of the components and the relations between the components and we try to determine the properties of the compound, then – if chemical compounds are truly emergent – we are bound to fail. Our failure is not due to some mysterious chemical spirits similar to the *élan vital* in biology; for Broad, the natural kinds that are the subject matter of chemistry are wholly composed of the kinds that are the subject matter of physics. Nor is it necessarily due to the lack of precise knowledge of the initial conditions or computational power. Rather, the problem is more fundamental – the “unique and ultimate” character of the laws of chemistry (Broad 1925, p. 65). Such laws, which connect the properties of chemical compounds with the properties of their components are called by Broad trans-ordinal laws. According to Broad, our failure is due either to (i) the existence of innumerable “latent” properties in each element, each of which is manifested only in certain conditions, or (ii) to the lack of any general principle of composition, such as the parallelogram law in dynamics, by which the behaviour of any chemical compound could be deduced from its structure and from the behaviour of each of its elements in isolation (Broad 1925, pp. 66–67).

McLaughlin interpreted Broad (or more generally British emergentism) as holding the view that an emergent whole possesses force-generating properties of a sort not possessed by any of its parts (McLaughlin 2008, p. 41). On this view, when particles are arranged in certain select configurations, new, unanticipated forces arise. McLaughlin called these forces *configurational*.⁷ In chemistry, configurational forces are supposed to be *sui generis* chemical forces characterizing the compounds, irreducible to physical forces characterizing the components. They are supposed to be capable of downward causation – the ability to influence the basal conditions from which they arise (i.e., the underlying dynamics). It is perhaps natural to think that on Broad’s view these forces may be responsible for the failure of compositionality and the emergent behaviour of chemicals, including chemical affinity. McLaughlin contrasted configurational forces with resultant forces, i.e., non-emergent forces which are generated by other forces, not by configurations of particles. “Emergence”, therefore, has been contrasted with “resultance”.

⁷ Although Broad does not use this term, McLaughlin (2008) interprets Broad in this way. According to McLaughlin, “it is clear that he [i.e., Broad] maintains that certain structures of chemical compounds can influence motion in fundamental ways” (McLaughlin 2008, p. 47).

McLaughlin finds the kind of emergentism espoused by Broad “enormously implausible”. According to McLaughlin, the fall of British emergentism was not caused by some philosophical difficulties, but by advances in science:

[Q]uantum mechanical explanations of chemical bonding in terms of the electro-magnetic force [...] render the doctrines of configurational chemical [...] forces enormously implausible. (McLaughlin 2008, p. 49)

McLaughlin’s view has been widely embraced by philosophers. It would not be too exaggerated to say that it has become the orthodoxy amongst contemporary philosophers. But this orthodoxy has been challenged by Scerri (2012) who questioned the idea that progresses in theoretical physical chemistry have dealt a death blow to Broadian emergence. Scerri argues that today’s theories of bonding still do not allow us to predict in advance the properties of compounds based on the properties of the components. Indeed, in all but the simplest cases, the theoretical and computational difficulties are enormous. But Scerri does not believe that this warrants one to draw the conclusion that emergence as conceived by Broad is a genuine phenomenon. Rather, Scerri distinguishes between what he calls “apparent emergence” (i.e., epistemic emergence, which might occur because of the limitations of our current theories) and “ontological emergence” (i.e., a deeper kind of emergence, which might occur because of the reasons presented by Broad). It is not hard to argue that chemistry does exhibit some sort of epistemic emergence, but according to Scerri it is an open question whether it exhibits ontological emergence as well.

Broad’s account of emergence has inspired a prominent contemporary account of ontological emergence in chemistry, due to Hendry (2003, 2006, 2010a, b, 2012). Instead of employing configurational forces, Hendry employs “configurational Hamiltonians” – non-resultant Hamiltonians governing the behaviour of the molecule. Hendry gives as an example the CO₂ molecule. One can view the parts of this molecule as quantum mechanical harmonic oscillators and rigid rotators. But one can do this only after one assumes the linear structure of CO₂. Where does this assumed molecular structure come from? Hendry argues that rather than deriving this structure using resultant Hamiltonians, the linear structure of CO₂ is put in “by hand”. For Hendry, this is tantamount to assuming “configurational Hamiltonians”. Since the overall molecular structure constrains the motions of the parts of the molecule, this would count as an example of downward causation.

Now, the reductionist may agree that the molecule as a whole constrains the motion of its parts. But he may still disagree that this is a genuine case of downward causation; the reductionist may say that the powers of the molecule to constrain the motion of its parts come ultimately from the parts themselves, and their inter-relations. We use the configurational Hamiltonians, the reductionist may argue, just because the real (resultant) Hamiltonians are just too hard to obtain. Thus, the configurational Hamiltonians are just approximations to the real (resultant) Hamiltonians, and their adoption does not make much of a difference. But Hendry argues this answer won’t work. Hendry starts by pointing out that in the calculation of the wavefunction of the molecule one makes use of the Born-Oppenheimer approximation, which allows the molecular wavefunction to be broken into its electronic and nuclear components, and in which the nuclei are considered

“clamped”. But following Woolley and Sutcliffe (1977), Hendry argues that in the process of applying the Born-Oppenheimer approximation, the symmetry properties of the molecular wavefunction are removed (Hendry 2010a, b). The idea here is that quantum mechanics cannot recover the structure (and the lower symmetry) of real molecules. For example, in the case of isomers, quantum mechanics cannot distinguish between two different molecules, for it assigns the same wavefunction to two distinct molecular structures – a wavefunction which is in fact a superposition of the wavefunctions corresponding to the two definite molecular structures (and has thus a higher symmetry). Hendry suggests that just as the measurement problem in quantum mechanics cannot be solved by a “superposition approximation” (i.e., simply discarding the part of the wavefunction that does not correspond to what is observed), it is just as much a mistake to invoke the Born-Oppenheimer approximation to argue that the structure of molecules is determined by resultant, albeit hard to obtain Hamiltonians.

In reply to Hendry’s arguments, Scerri (2012) has pointed out that the lower symmetry of the molecules can be accounted for by their quantum-mechanical interaction with the environment (decoherence). Molecules are never in isolation; they are always surrounded by other molecules, to which they interact. Consequently, the wavefunction of a given molecule will not be for a long time in a superposition of states corresponding to two different molecular structures. The idea here is that pretty fast, the superposition will collapse and the molecule will assume the observed structure. Scerri claims that “taking account of quantum decoherence allows one to tame the effect of entanglement and appears to alleviate the concern that ontological entities such as molecules with particular structures might not exist in their own right” (Scerri 2012, p. 20).

The appeal to decoherence is an interesting move, but it is not without its problems. First, it should be mentioned that decoherence does not solve the problem of definite outcomes, which together with the problem of the preferred basis forms the so-called measurement problem in the foundations of quantum mechanics (Adler 2003; Zeh 2003). Decoherence just passes the entanglement on to the environment. In fact, decoherence exacerbates the measurement problem. Scerri recognizes that decoherence does not allow one to predict any particular outcomes. But he claims that this concern can be addressed by assuming that the collapse is ubiquitous, and it happens even in the absence of observers. He claims that this intuition is supported by the fact that the classical world is populated by definite outcomes (i.e., definite outcomes are not just an effect of conscious observers). But these remarks essentially amount to taking a stand on the interpretation of quantum mechanics; of course, they do not by themselves amount to an interpretation of quantum mechanics, but they favour a set of interpretations over others. So it looks like that the debate about configurational Hamiltonians and molecular structure has become entangled with the problem of interpreting quantum mechanics. Thus, it seems that to elucidate the hard problem of emergence in chemistry one needs to elucidate a perhaps even harder problem. Since there is the risk that this debate could degenerate into a debate about the proper interpretation of quantum mechanics or even turn into a stalemate, perhaps it is worth considering a different approach to emergence in chemistry.

Insofar as Hendry's theory of emergence focuses on entities, it is at odds not only with reductionism, but also with the causal closure or completeness of physics – the thesis that “all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws” (Papineau 1990, p. 67). This is because on Hendry's view, molecules are capable of downward causation. So if the theory of emergence advocated by Hendry is true, the set of physical causes must be supplemented with *sui generis* chemical causes – molecules exerting downward causation on their parts.

The rejection of the causal closure of physics entailed by the kind of ontological emergence advocated by Broad and Hendry may be problematic. Some philosophers argued that the causal closure of physics is supported by inductive arguments based on the history of science (Papineau 2002, see Appendix) or on conservation laws (Vicente 2006).⁸ One worry is that in a world in which all basic forces are physical and the conservation of energy is respected, *sui generis* non-physical forces (whatever this might mean) of the kind required to break the causal closure of physics could not arise. Maybe this objection can be responded to, and maybe the causal closure of physics is just another philosophical preconception of the naturalistic-minded philosopher. Or maybe not. Regardless, it seems to me that it would be preferable if the ontological autonomy of chemistry did not depend on a theory of emergence which is committed to the falsity of the causal closure of physics. This is another reason why it may be fruitful to approach emergence in chemistry differently.

Scerri's view on the current state of affairs regarding emergence in chemistry is that just as McLaughlin has failed to rule out emergence and downward causation, so Hendry has failed to make a case in their favour. Scerri believes that the proper attitude to adopt towards emergence and downward causation in chemistry is agnosticism. Given the points I made earlier (about how the debate over the kind of emergence defended by Hendry might require one to take a stand on the interpretation of quantum mechanics, and about how the rejection of the causal closure of physics that it entails might be at odds with the principle of the conservation of energy), but also given what is at stake (namely the disciplinary autonomy of chemistry), I think it is worth investigating alternate routes to emergence. The rest of this paper sketches such a proposal.

4.3 A Novel Approach: Functional Emergence

Before sketching the contours of a new approach to emergence in chemistry it would be useful to state why such an account is desirable and what we want from it. As mentioned in the introduction, developing accounts of emergence in chemistry is important because emergence can help us defend the ontological autonomy

⁸ For a different view, see Gibb (2010).

of chemistry. The question that I think needs to be taken seriously is this: if the entities that chemistry talks about are composed of nothing but the entities that quantum mechanics talks about, why do we have chemistry and not just applied quantum mechanics? Are there any good reasons for upholding the ontological autonomy of chemistry, as opposed to just a merely epistemic, methodological or historical autonomy? If the kind of stuff chemistry talks about consists of the kind of stuff that quantum mechanics talks about, what justifies belief in chemical properties, or that in chemical laws or explanations? Are there even *chemical* properties, laws, and explanations, as opposed to just complex quantum-mechanical properties, laws, and explanations? Does chemistry latch onto genuine features of the world, which inhabit a distinct ontological level? Or rather the chemical properties and laws are just useful instruments for predicting and explaining, but ultimately with no claim to the fundamental truths about nature, which remain microphysical? If chemistry is emergent, then these questions may find satisfactory answers. If one can show that there really are *chemical* entities, properties, laws and explanations, then the ontological autonomy of chemistry can be secured.

So far, the philosophical efforts towards a theory of ontological emergence in chemistry focused on the emergence of entities. For Broad, what was emergent was chemical compounds; for Hendry, what is emergent is molecules (molecular structure). But an ontology contains more than just entities; it also contains processes, properties, phenomena, laws, and on some understandings of ontology, even explanations. All these are just as legitimate elements of an ontology as entities. The approach I am proposing focuses not on entities, but on properties and laws, which can be used in *sui generis* chemical explanations. It starts from the observation that many chemical properties are defined not in terms of their constitutive microphysical structure, but functionally, in terms of their efficient roles. In particular, many chemical properties are defined by their behaviour in relation to other chemical properties, in the context of chemical reactions. The idea that a thing is defined by what it does and not by what it consists of was first advocated by Alan Turing, in the foundations of computer science and artificial intelligence (Turing 1950). Turing thought about it via an analogy with the mathematical concept of a function (1950, p. 439). Turing's idea was quickly adopted in the philosophy of mind, where it served as a basis for an alternative theory of mind, different from both the identity theory and behaviourism (Putnam 1975a, b; Fodor 1974). The theses of functionalism and multiple realizability have also inspired anti-reductionist arguments in the philosophy of biology (Kitcher 1984, 1999; Kincaid 1990). But chemistry is, I believe, the ideal domain where this sort of anti-reductionist argument can be made. The fact that chemical properties can be intersubjectively scrutinized, that they are amenable to measurement, experiment and to a quantitative understanding to a greater extent than those in the other special sciences makes chemistry one of the best case studies (see also Scerri and McIntyre 1997, p. 227; Humphreys 1997b). Chemistry is the discipline that is in some sense closest to physics, and therefore it is the first domain outside physics itself where we can observe functional properties and irreducibility/emergence, if these truly exist.

The approach to emergence I'm proposing starts from the observation that many chemical properties are defined not in terms of their constitutive microphysical structure, but functionally, in terms of their efficient roles. So far, philosophers of

chemistry have not given appropriate consideration to this idea. For example, the volume which was published as a result of the 3rd Erlenmeyer Colloquy for the Philosophy of Chemistry, titled “The Autonomy of Chemistry” does not even mention chemical functional properties, despite the broad consensus and shared anti-reductionist attitudes among the participants (Janich and Psarros 1998). In fact, the idea of multiple realizability (which is often associated with functionalism) has been regarded with distrust in the philosophy of chemistry, being labelled as “wishful thinking” (Scerri 2000). Yet, multiply realizable properties feature prominently in the discussions about the limits of reductionism in philosophy of mind, philosophy of biology, and philosophy of physics (Batterman 2000, 2002). I think chemistry makes no exception; on the contrary, I think chemistry provides us with some of the best examples of functional, multiply realized properties.

Consider the property of being an acid. On the Arrhenius definition, acids are defined as those substances which, when dissolved in water, increase the concentration of hydrogen ions in the solution. On the Brønsted-Lowry definition, an acid is any compound that can donate one or more protons to other chemical species in chemical reactions. And on the Lewis definition, acids are those compounds that accept a pair of electrons from another compound in a chemical reaction. All these definitions are functional, i.e., they pick out acids not by referring to their microphysical structure, but by referring to their behaviour in relation to other chemical substances. Compare the property of being an acid with the property of being an alcohol. Alcohols are those molecules that have a hydroxyl group bound to a saturated carbon atom. This microstructural commonality can be invoked when explaining the chemical properties of alcohols. In a certain sense of the term “reduction”, the property of being an alcohol reduces (i.e., is identical) to the property of being a microphysical system containing a hydroxyl group bound to a saturated carbon – all alcohols and only alcohols have this microstructural property. But the property of being an acid (or, more accurately, acidity in general) does not “reduce” in a similar manner to any given microstructural property. Of course, one may accept that any given instance of an acid (or acidic behaviour) is identical with a given instance of a physical property or process – token reductionism may hold. But acidity as such (as a property type) cannot be identified to any given microstructural property – type reductionism fails. Acidity is first and foremost a behaviour, which can be realized by many systems of electrons and nuclei. In philosophical lingo, the property of being an acid is said to be *multiply realized*. Because of this, it is not discernible at the lower level as a microstructural property. It “emerges” out of the microphysics, and becomes visible only in the context of a chemical reaction, as a pattern of chemical behaviour.

Acidity may not be the only functional property in chemistry: arguably, the property of being a base, a reductant, an oxidant may also be functional. To these, one may add the property of being a metal. More than 70 % of existing chemical elements are metals; at standard conditions of temperature and pressure, 91 elements out of 117 are considered metals. Twelve out of 18 groups in the periodic table are occupied exclusively by metals – alkali elements, alkaline earth elements, lanthanides, actinides, and the transition elements, are all metals. Some elements in group 13 to group 16 are metals too. As one can expect, the microstructural description for all these atoms will look disunified. Finding a microstructural

feature that is shared by all metal atoms and only by them is highly implausible. Despite the fact that their microstructural descriptions are wildly heterogeneous, metals have interesting chemical properties in common: their atoms readily lose electrons to form positive ions; they form metallic bonds with other metal atoms and ionic bonds with nonmetal atoms. Since the property of being a metal is not characterized by a shared microstructure, but by what the entities instantiating the property can do, this property is also functional.

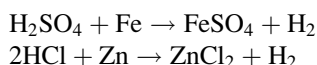
Functional properties in chemistry are not only multiply *realized* (in the sense of there being many systems composed of electrons and nuclei that can carry out the specified role), but they are also multiply *realizable* – the list of systems composed of electrons and nuclei that can carry out the specified role is open ended. Chemistry is in the business of synthesising new substances. Although synthetic elements have also been created, most of the synthetic substances are compounds. For any functionally defined chemical property like acidity, chemists can come up with new compounds which can carry out that behaviour.

If there are functional, multiply realizable properties in chemistry, then this means that certain notions of reductionism cannot be maintained. I have already mentioned type reductionism. Type reductionism (or, as Fodor called it, “type physicalism”) is the idea that every property mentioned in the laws of any science is a physical property. If type reductionism were true, there would be a one-to-one correspondence between chemical properties and microstructural properties. The kinds that chemistry talks about would be shown to be identical to, or at least coextensive with, physical kinds. For some chemical properties (like the property of being an alcohol) this is in fact true – as stated, there is a one-to-one correspondence between alcohols and microphysical systems containing a hydroxyl group bound to a saturated carbon atom. But for other chemical properties (like the property of being an acid) it is not. This suggests that properties like acidity are not physical properties in disguise; they are *sui generis* chemical properties, i.e., chemical properties in their own right. Acidity is made possible by physical processes at the lower level, and any instance of acidic behaviour (i.e., any particular reaction) may be identical to (or coextensive with) a specific physical process at the lower level. But acidity as a property *type* is not identical to (or coextensive with) any microstructural physical property. It emerges as a property only when one zooms out of microphysics and starts looking not at microphysical structures, but at their behaviours.

The existence of functional properties in chemistry also impacts reductionism about chemical laws. On Nagel’s concept of reduction (1961), chemistry would reduce to physics if one could derive all the laws of chemistry from the laws of physics together with bridge laws connecting the terms in the vocabularies of the two sciences.⁹ The philosophical literature on Nagelian reduction has long debated

⁹ In this context, by “chemical laws” I do not mean exceptionless and timeless universal truths, of the kind that occur in fundamental physics (or maybe not even there). Rather, I mean the kind of regularities chemists use on a daily basis, and which chemistry students find circled in chemistry textbooks. For example, the statement that “Acids in reaction with metals generate hydrogen gas” would count as a chemical law. If one does not accept this charitable reading of what a law should mean, then the Nagelian reduction of chemistry to physics cannot even begin to be discussed.

the implications of multiple realizability for bridge laws. If one conceives of bridge laws as a posteriori identity statements, then bridge laws must be biconditionals linking kinds. That is, they must connect a chemical kind with exactly one micro-physical kind.¹⁰ Multiple realizability prevents this one-to-one connection.¹¹ But even if the reductionist retreats to a one-to-many connection between a chemical property and a heterogeneous set of physical properties, it is still unclear that the desiderata of Nagelian reduction can be met. As mentioned, the reduction of chemistry requires the derivation of chemical laws from physical laws. But it is questionable that the relationship between the physical realizers of the functional properties which figure in some chemical laws would have any nomic character. Consider the chemical law that acids in reaction with metals generate a metal salt and hydrogen. The number of compounds rendering this chemical law true is vast. Take the following two examples (in aqueous solution):



Now, to paraphrase Fodor (1974), one may say that while it is a law that sulfuric acid in reaction with iron produces iron sulfate and hydrogen, and it is a law that hydrogen chloride in reaction with zinc produces zinc dichloride and hydrogen, it is not a *law* that either sulfuric acid or hydrogen chloride in reaction with either iron or zinc produces either iron sulfate and hydrogen, or zinc dichloride and hydrogen. This last statement is too gerrymandered to have any nomic character. Nonetheless, the more general claim, asserting that acids in reactions with metals produce a metal salt and hydrogen, is a law. Even if the two statements above expressing the reactions can be construed as stating laws of physics (which is in itself problematic), one could not use them to deduce the chemical *law* that acids in reaction with metals generate a metal salt and hydrogen. Since the nomic character of this statement (and of similar statements relating functional properties) cannot be recovered from the reduction base, such statements – if laws at all – must be regarded as *sui generis* chemical laws.

The functional, multiply realizable chemical properties may occur in higher level chemical explanations. Q: “Why did the marble antefixes on the roof the Philadelphia Merchants’ Exchange lose their detail?” A: “Because of the acid rain.” I take it that this is a perfectly satisfactory explanation. The answer successfully selects one of the contrast classes (chemical) and eliminates the others (mechanical, temperature variations, etc.). Admittedly, the explanation is not specific; it does not mention the precise composition of the acid rain, and it leaves out the specific chemical reactions. But this is not necessarily a defect of the explanation; in fact, it

¹⁰ I am assuming a strong connection between kinds and properties.

¹¹ Of course, one may reply by saying that bridge laws need not be biconditionals. But there are many problems with this move, and this is not the place to discuss them. I will just mention Fodor who writes that if the relation in the bridge law “is interpreted as any relation other than identity, the truth of reductivism will only guaranty the truth of a weak version of physicalism” (1974, p. 99).

can be a virtue. By not going into the details, the explanation is *unified*: it sees various compounds as instances of a single kind of substance, namely acid. Since the explanation is insensitive to the particular compounds responsible for the acidic properties of the rain, it is *robust*: it remains valid despite variations in the composition of the acid rain that may occur from year to year. Also, the explanation has a *broad explanatory range*: it can account for the loss of detail in the marble antefixes on buildings situated in different geographical locations, where the acid rain has a different chemical composition. Since it features a *sui generis chemical* property, the explanation above may be called a *sui generis chemical* explanation. In contrast with the explanations mentioning the particular reactions (which perhaps could be seen by a ruthless reductionist as physical explanations), the explanation invoking the acidity of the rain is robust, unified, and has a broad explanatory range. But this happens only because it is a higher level explanation, i.e., an explanation which employs a higher level concept.

If chemical properties, laws and explanations are not identical or coextensive with physical properties, laws and explanations, then they should be treated as *sui generis*. The existence of *sui generis* chemical properties, laws and explanations supports the idea that chemistry is ontologically autonomous from physics, which is one of the two defining characteristics of emergence. The other characteristic of emergence, namely dependence, is also satisfied by the account I'm proposing. The functional chemical properties like acidity are made possible by the physical processes involving systems of electrons and nuclei. The kind of emergence I'm proposing has no problems embracing *supervenience physicalism* – the idea that any physical duplicate of our world is a duplicate of our world simpliciter. I take the following to be true: (i) if the microphysical level were to disappear, the chemical level would disappear as well; (ii) any change at the chemical level must involve a change at the microphysical level; (iii) any microphysical duplicate of our world will be a chemical duplicate.

Since the view I'm proposing meets both characteristics of emergence, and is made possible by the existence of functional properties, I will call it *functional emergence*. The use of the term "emergence" is appropriate because the existence of functional properties in chemistry supports the layered view of the world characteristic of emergentism. The *sui generis* chemical properties, laws and explanations function at a higher level than the physical properties, laws and explanations; they depend on the physical level, but they do not reduce to it.

I take it that supervenience physicalism is an uncontroversial thesis, which can be shared by reductionists and emergentists alike. But, as mentioned earlier, not all versions of emergence share a deeper physicalist commitment, namely the completeness of physics. For example, those versions of emergence which are committed to the emergence of entities (e.g., Broad's or Hendry's) will conflict with the thesis that all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws. For if there are *sui generis* chemical entities which are capable of causing physical events (via downward or horizontal causation) then the causes of those events won't be strictly speaking physical; they will be *chemical*. But functional emergence does not take this step. On the view that I'm proposing, entities may be wholly resultant.

Functional emergence need not be committed to the emergence of entities, or to their ability to exert downward causation; it is committed solely to the emergence of properties, laws, and explanations. As a result, there need not be any conflict with the completeness of physics; functional emergence and the completeness of physics can peacefully coexist.

4.4 Two Objections

There are several problems with the view that I'm sketching, but I will only discuss two of them. First, one may object to calling the account of emergence I'm proposing *ontological*. Since on this account entities do not count as emergent, why claim that functional emergence is a kind of ontological emergence? After all, if all chemical entities are composed of nothing else except microphysical entities, doesn't this mean that the ontology of chemistry reduces to, or is a subset of, the ontology of physics?

The problem with the argument above is that it construes ontology in a restricted way, as referring exclusively to entities (i.e., individuals). Ontology is concerned not only with entities, but also with properties, laws, and on some accounts, explanations. If one distinguishes between a property and its instances, as one should, the fact that every instance of a chemical property is composed of nothing else except instances of microphysical properties does not mean that all chemical properties are in fact microphysical properties in disguise.¹² Similarly, it would be a mistake to think that if all events are governed by physical laws, then all laws must be physical. Although the entities that chemistry talks about may be composed of nothing else except microphysical entities, this leaves open the possibility of *sui generis* chemical *properties* and *laws*. But if that is the case, there is a sense in which one can still talk about the ontological autonomy of chemistry. This result contrasts with the view advocated by McIntyre, who argued that the ontological interpretation of the concept of emergence should nearly always be eschewed in favour of an epistemological interpretation (McIntyre 2007).

It must be admitted, however, that this ontological autonomy is not radical: if the entities that microphysics talks about were to vanish, there would be nothing left; consequently, there would be no chemical properties, no laws relating these properties, and no explanations employing those laws and properties; although the ontology of chemistry is autonomous from the ontology of physics, it relies upon it.

The second problem is that not all chemical properties are defined functionally. What does this situation tell us with respect to the nature of chemistry as a science, and its autonomy from physics? In my view, this situation reflects the status of chemistry as "the first" of the special sciences. Some chemical properties (like the property of being an alcohol) can be reductively identified with microphysical

¹² For the distinction between a property and its instances see Swoyer and Orilia (2011).

properties. But others (like being an acid), are defined functionally, and they will not be reducible to any particular physical properties. This depicts an image of chemistry as a “mixed” science – a science that is close enough to physics so that some of the properties it talks about are microphysical properties, but also a science that begins to emancipate itself from the base, and deals with genuinely new properties. The “mixed” character of chemistry qualifies the thesis that chemistry is ontologically autonomous from physics, and perhaps it weakens it to some extent. Nonetheless, it would be wrong to conclude that the mixed character of chemistry makes the ontology of this discipline as a whole a sub-domain of the ontology of physics. Since the *sui generis* properties and regularities that chemistry talks about are sufficiently numerous and pervasive, the ontological autonomy of chemistry can be preserved.

This image of chemistry as a “mixed science” offers only a partial support to the classical layer cake model of science that has been assumed by many reductionists, anti-reductionists and emergentists alike. The chemical properties and regularities are always susceptible of disruptions “from below”. In other words, chemical properties and regularities can always be affected by physical or microphysical factors. A clear example is the influence of temperature on chemical reactions, but numerous other examples could be found. Physical factors such as electromagnetic fields, pressure, even gravity may interfere with chemical properties and laws, no matter how *sui generis* these are. Thus, although chemistry has its own ontology which is distinct from that of physics, is not “insulated” from physics. To express this in the terms of the layer cake metaphor, chemistry is not a perfectly distinct layer that lays flat on top of the physical layer. Instead of the layer cake model, perhaps a better model could be suggested, one which captures more accurately the relationships between the various sciences. For the lack of a better metaphor, this could be called the “Easter bread” model. In the “Easter bread” model, the sciences are not arranged neatly in distinct layers, with physics at the base and then followed by chemistry, biology, psychology, etc.; rather, they interweave and penetrate each other globally, although locally they typically retain their distinctness.

4.5 Conclusion

In this paper I attempted to outline a novel approach to emergence in chemistry. The motivation for this was twofold: on the one hand, emergence is a way to secure the ontological autonomy of chemistry from physics; on the other, the most prominent approaches to ontological emergence in chemistry have been met with scepticism. The account I proposed differs from the most prominent existing accounts in several ways. What is emergent on my account is not entities, but properties, laws and explanations. Although the account I’m proposing may be new to chemistry, it is not new to philosophy (though the phrase “functional emergence” as I used it here may be). Functional properties which are multiply realizable have long been associated with a philosophical position known as nonreductive

physicalism. Like emergence, nonreductive physicalism attempts to reconcile physicalism with the idea that the special sciences are not reducible to physics.

The account I proposed here amounts to little more than a sketch. There are still many important questions to be answered, and many of its aspects need to be elaborated in more detail. The arguments I used here need to be improved and expanded; many imperfections need to be ironed out; in one word, a lot of work remains to be done. But the broad outlines I sketched here are, I think, essentially correct.

References

- Adler SL (2003) Why decoherence has not solved the measurement problem: a response to P. W. Anderson. *Stud Hist Philos Mod Phys* 34B:135–142
- Batterman RW (2000) Multiple realizability and universality. *Br J Philos Sci* 51:115–145
- Batterman RW (2002) *The devil in the details: asymptotic reasoning in explanation, reduction, and emergence*. Oxford studies in philosophy of science. Oxford University Press, Oxford
- Broad CD (1925) *The mind and its place in nature*. Harcourt, Brace & Company, Inc, New York
- Fodor JA (1974) Special sciences (Or: the disunity of science as a working hypothesis). *Synthese* 28(2):97–115
- Gibb S (2010) Closure principles and the laws of conservation of energy and momentum. *Dialectica* 64(3):363–384
- Hendry RF (2003) Chemistry and the completeness of physics. In: Rojszczak A, Cachro J, Kurczewski G (eds) *Philosophical dimensions of logic and science*. Kluwer, Dordrecht, pp 165–178
- Hendry RF (2006) Is there downward causation in chemistry? In: Baird D, Scerri E, McIntyre L (eds) *Philosophy of chemistry. Synthesis of a new discipline*. Springer, Dordrecht, pp 173–189
- Hendry RF (2010a) Chemistry: emergence vs. reduction. In: Macdonald C, Macdonald G (eds) *Emergence in mind*. Oxford University Press, Oxford, pp 205–221
- Hendry RF (2010b) Ontological reduction and molecular structure. *Stud Hist Philos Mod Phys* 41:183–191
- Hendry RF (2012) Reduction, emergence and physicalism. In: Hendry RF, Needham P, Woody A (eds) *Handbook of the philosophy of science. Volume 6: philosophy of chemistry*. Elsevier, Amsterdam, pp 367–386
- Humphreys P (1996) Aspects of emergence. *Philos Top* 24:53
- Humphreys P (1997a) Emergence, not supervenience. *Philos Sci* 64:S337–S345
- Humphreys P (1997b) How properties emerge. *Philos Sci* 64(1):1–17
- Janich P, Psarros N (1998) *The autonomy of chemistry: 3rd Erlenmeyer-Colloquy for the Philosophy of Chemistry*. Konigshausen & Neumann, Würzburg
- Kim J (2006) Emergence: core ideas and issues. *Synthese* 151(3):547–559
- Kincaid H (1990) Molecular biology and the unity of science. *Philos Sci* 57(4):575–593
- Kitcher P (1984) 1953 and all that. A tale of two sciences. *Philos Rev* 93(3):335–373
- Kitcher P (1999) The hegemony of molecular biology. *Biol Philos* 14:195–210
- Llored J-P (2012) Emergence and quantum chemistry. *Found Chem* 14:245–274
- Lombardi O, Labarca M (2005) The ontological autonomy of the chemical world. *Found Chem* 7(2):125–148
- Luisi PL (2002) Emergence in chemistry: chemistry as the embodiment of emergence. *Found Chem* 4:183–200

- Manafu A (2013a) Concepts of emergence in chemistry. In: Llored J (ed) *Philosophy of chemistry: practices, methodologies and concepts*. Cambridge Scholars Publishing, Newcastle upon Tyne, pp 659–674
- Manafu A (2013b) Internal realism and the problem of ontological autonomy: a critical note on Lombardi and Labarca. *Found Chem* 15(2):225–228
- McIntyre L (2007) Emergence and reduction in chemistry: ontological or epistemological concepts? *Synthese* 155:337–343
- McLaughlin B (2008) The rise and fall of British emergentism. In: Bedau A, Humphreys P (eds) *Emergence. Contemporary readings in philosophy and science*. MIT Press, Cambridge, MA
- Mill JS (1882) *A system of logic, ratiocinative and inductive: being a connected view of the principles of evidence and the methods of scientific investigation*. Harper and Brothers, New York
- Nagel E (1961) *The structure of science: problems in the logic of scientific explanation*. Harcourt, Brace & World, London
- Papineau D (1990) Why supervenience? *Analysis* 50:66–71
- Papineau D (2002) *Thinking about consciousness*. Oxford University Press, Oxford
- Putnam H (1975a) Minds and machines. In: Putnam H (ed) *Mind, language, and reality*, vol 2, *Philosophical papers*. Cambridge University Press, Cambridge
- Putnam H (1975b) The nature of mental states. In: Putnam H (ed) *Mind, language, and reality*, vol 2, *Philosophical papers*. Cambridge University Press, Cambridge
- Putnam H, Oppenheim P (1958) The unity of science as a working hypothesis. *Minn Stud Philos Sci* 2:3–36
- Scerri E (2000) The failure of reduction and how to resist disunity of the science in the context of chemical education. *Sci & Educ* 9:405–425
- Scerri E (2012) Top-down causation regarding the chemistry-physics interface: a sceptical view. *Interface Focus* 2:20–25
- Scerri E, McIntyre L (1997) The case for the philosophy of chemistry. *Synthese* 111:213–232
- Swoyer C, Orilia F (2011) Properties. In: Zalta EN (ed) *The Stanford encyclopedia of philosophy*. Winter 2011 edition
- Turing AM (1950) Computing machinery and intelligence. *Mind* 59(236):433–460
- Vicente A (2006) On the causal completeness of physics. *Int Stud Philos Sci* 20(2):149–171
- Woolley R, Sutcliffe B (1977) Molecular structure and the Born-Oppenheimer approximation. *Chem Phys Lett* 45:393–398
- Zeh H (2003) Basic concepts and their interpretation. In: Giulini D, Joos E, Kiefer C, Kupsch J, Stamatescu I-O, Zeh HD (eds) *Decoherence and the appearance of a classical world in quantum theory*. Springer, Berlin