Smaller Than A Breadbox: Scale and Natural Kinds

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1 Introduction

Suppose I have a collection of a few billion billion gold atoms. If the atoms in the collection are grouped together into one massive lump, the result looks yellow and shiny and, if left undisturbed in an office, it will do very little (besides fluctuating in value over time on the stock market). Heating this lump above 1064° C will, under atmospheric conditions, produce a molten puddle. With the appropriate metalworking tools, the lump may be rolled into the shape of a ring or smashed into the shape of a coin. The electrons in the atoms in the lump are delocalized, spreading among many nuclear centers. The lump will resist corrosion and rusting, and it will be more chemically inert than similarly-proportioned lumps of metal made up of zinc or lithium atoms.

However, if I rearrange the atoms in my lump into clusters of a few hundred atoms each, all these properties change. In order to preserve this new arrangement of atoms, the clusters will need to be suspended in a carefully-prepared solution that has been designed to fight the forces of surface tension, chemical kinetics, and thermodynamics so that the clusters will not coagulate back into one massive lump. The individual clusters in this solution have physical properties, such as conductivity and ductility, that differ from the physical properties of the lump and which change depending on the size, shape, and surface chemistry of the clusters. Collectively, the clusters appear differently-colored than the shiny, yellow lump: out of solution the group of clusters has the dull, reddish-black appearance of river mud; in solution, the clusters turn a previously-clear liquid red or brown, a color brought about not by normal pigmentation but instead by a rare optical phenomenon known as localized surface plasmon resonance (LSPR). This phenomenon only occurs when the clusters are small enough that their diameter is shorter than the wavelength of visible light. And finally, in contrast to the big lump of gold, these clusters are catalytically active—that is, they can be used to speed up other reactions that are performed in solution with them.

At least one further case is possible, namely that my atoms are neither a lump nor a set of clusters, but are, simply, non-interacting atoms in a vacuum, with all and only their atomic properties: 79 protons, 79 neutrons and electrons, some electronic symmetries and characteristic dispositions toward bonding, but without any macroscopic properties whatsoever—no color, no temperature, no malleability or ductility. All this is to say that the macroscopic kindhood of my collection of gold atoms is underdetermined by solely specifying the identity of the atoms involved.¹

This underdetermination lies at the intersection of a variety of debates in philosophy of science and contemporary metaphysics, including debates about natural kinds, reduction, emergence, and the structure of scientific theories and explanations. Roughly put, the dilemma is this: either each of the three arrangements is a member of the same kind, in which case that kind class fails to pick out the macroscopic properties of any of the samples, or each of the arrangements is a member of a different kind, in which case atomic number is not the essential identity-conferring property of the samples. And on either horn of the dilemma, the question of the connection between microstructural similarity and macrostructural difference still remains.

The three samples in this case are not rare in being examples of microstructural similarity underdetermining macroscopic properties. Batterman [2] has recently introduced the literature to a case of a composite material made of a mixture of conductive and non-conductive substances. When "islands" of non-conductive material are mixed into conductive material, the result is a conductive composite, and *vice versa*. In Batterman's composite, as in my three arrangements of gold atoms, further information about higher-level structural features of a sample are needed to determine the macroscopic properties of the material. And the question remains: where in the move from microstructure to macrostructure should one draw the borders of kindhood?

In this article, I argue that at least in the case of scientific kinds, philosophical accounts of kindhood should be indexed to the length, time, or energy scales of the objects of a scientific investigation. Further, this indexing is not a result of mere pragmatic convention, but instead a consequence of a rather unassuming intuition that the structure of scientific concepts and theories

¹For those whose ontological proclivities favor desert landscapes, this underdetermination is not intended to imply any spooky metaphysics of collections. Rather, the underdetermination is meant to problematize the view that scientific theories and models can succeed in certain reductive frameworks, where the only objects populating models are the "most fundamental" elements of a theory. In other words, scientific practice proceeds via the use of the higher-level kind categories I discuss here, and my interest is in characterizing those kind categories in order to better understand their success in scientific settings.

should follow the structure of the systems they aim to represent, reference, and understand. That is, it is a scale-dependence in the systems themselves that provides opportunities and support for scale-dependent changes in the landscape of kinds under consideration in a lab. For my three samples of gold, the upshot is that I permit each of the samples to persist as a kind unto itself, but each is a different kind of kind than the next. Each kind is useful in different scientific settings because each picks out a kind whose properties of interest exist at a different scale from the others. Each scale makes possible a certain aspect of theory construction or experimental practice.

Physicists already have some semantic infrastructure to discuss how properties can group across different scales: the *characteristic length and time scales* of a system or object of theory or experiment pick out precisely this notion (cf. e.g. [22]). And recently, philosophers of physics have picked up on this infrastructure, building an intersection between physical discussions of characteristic scales and philosophical discussions of reduction, emergence, idealization, and explanation (cf. e.g. [1, 33, 7]. But their discussions have yet to result in an application of the concept of a characteristic length or time scale to debates about kindhood and substance identity; that fork of the intersection simply has yet to be taken. This essay marks a first step down that path.

I proceed as follows: In Section 2, I motivate the ensuing discussion by framing the problem of natural kinds within the context of contemporary philosophy of science, showing that while explicit discussions of kindhood have largely been confined to individual sciences (notably chemistry, biology, and psychiatry), the worries that underlie the natural kinds debate are in the background of a number of recent, prominent accounts of the structure of scientific theories and the shape of scientific progress. I focus in particular on Chang's Inventing Temperature [8] and Wilson's Wandering Significance [32]. In Section 3, I propose a theory of chemical kinds that hinges on an oft-overlooked feature of chemistry, namely that kind terms are often used to bridge across the characteristic length scales of chemistry. Section 4 extends this account to the problem of nanoscale kinds and shows why standard accounts of chemical kindhood either fail to account for the difference between the lump of gold and the collection of nanosclusters, or fail to pick out their relevant similarities. I argue that in order to carry out the projects of nanoscience, scientists need both to be able to distinguish the former case from the latter case and to draw a connection between the two cases. Section 5 contains brief summary remarks.

2 The Methodological Problem of Kinds

A useful if oversimplified way of understanding the contemporary natural kinds literature is to divide worries about kindhood into two related but distinct categories: the metaphysical problem and the semantic problem. Metaphysical worries about kinds concern questions about naturalness, ontology, and essences: Do natural kinds have essences? Can the possession of essences, or other criteria, be used to separate natural from conventional kinds? What sorts of things are kinds, if anything at all? Can kinds change over time? Semantic worries about kinds, on the other hand, primarily concern questions about kind terms: How is the reference of a kind term fixed? What happens in cases where a kind term's extension is underdetermined by its use history? Can the extension of a kind term change over time? Often, these two sorts of worries are combined: Are essences what fixes the reference of kind terms, or is it something else?

Many contemporary discussions of kinds, following those of Kripke and Putnam, fall within the purview of one or both of the metaphysical or semantic problem. But even without solving either the metaphysical or the semantic problem, there remains a third set of worries about kinds, framed around questions of direct interest to contemporary scientific practice. These worries concern questions of the success and apparent indispensability of kind terms as tools for carrying out scientific projects: What explains the success of the Periodic Table of Elements throughout changes in scientific understanding of the atomic nature of matter? When is it appropriate to use viability of crossbred offspring as a criterion for species demarcation, and when genetic overlap? When in the course of chemical explanation is it necessary to specify qualities of a chemical bond (e.g. ionic vs. covalent, polarity, length, angle), and when is it sufficiently explanatory to refer to the presence or absence of a bond? These are questions about how kinds inform the practices of science, rather than questions about how science can inform theories of kinds. While different answers to the metaphysical or the semantic problem will influence one's response to questions such as these, none of these questions can be replaced by entirely metaphysical or semantic concerns. The aim of this section is to show that these methodological worries about the success of kinds in science comprise the central problem of kinds in philosophy of science, namely, how classification aids the aims and methods of science.

In philosophy of science, the metaphysical problem is often answered with a quietistic rejoinder,

by listing cases where classification continues to occur successfully in the absence of a specification of essence, or even in the absence of an answer to the essentialism question. This response can be seen especially in projects in the philosophy of biology, where kindhood is argued (e.g. by [13]) to be conferred by the history of a species or phylum, rather than by a shared, eternal essence. Even in cases of kinds typically thought to be essence-based, such as *gold* and *electron*, essences are not indisputably accepted.² Likewise, in philosophy of science the semantic question is often reframed in terms of the ability of scientists to refer to individual substances or species over time, coupled with stories of how realization of failures of reference (e.g. "phlogiston," "brontosaurus") led to scientific advance. So while there are many interesting responses to metaphysical and semantic questions in philosophy of science, a third category of worry about kinds underlies most writing about kinds in philosophy of science. I call this worry "the methodological problem of kinds." It is the endemic problem of kinds for philosophy of science.

Surveying discussions of kinds in philosophy of science reveals a recent and somewhat tentative consensus: whether or not kinds are natural, and whether or not they have essences, and whether or not the extensions of kind terms change on Pluto or Twin Earth, what kinds are are tools that scientists use to carry out the practice of science. From the problem of species classification in biology to the development of the Standard Model of Particle Physics, kinds are useful to science insofar as they can help scientists to determine how to proceed in carrying out an experiment, confirming a theory, or explaining a set of natural phenomena. The basic motivation behind theories as diverse as Boyd's homeostatic property clusters and Hacking's pragmatic theory of kindhood is a shared one, namely to determine how classification aids the practice of science.

This motivation for studying kindhood through a philosophy-of-science lens also appears in philosophical discussions of kinds in contemporary metaphysics and epistemology more generally, such as Millikan's On Clear and Confused Ideas [18]. While it is clear that Millikan does not endorse the methodological approach to kindhood as a path to understanding substance concepts, her acknowledgement of this function of kinds in science is nonetheless apparent:

When confidence is lost in the reality of a substance or in the univocity of a substance term, it may begin to be used in a strictly classificatory way. For example, terms for

²For instance, see Boyd [3] or Needham [20], for discussions of the absence of microstructural essences in chemical and other scientific kinds.

many mental disorders have vacillated over the years between being understood as capturing substances, naming single diseases for which single etiologies and therapies might eventually be discovered, and as being merely classificatory, defining useful groupings of symptoms for efficient transfer of information.

[18, p. 39]³

This motivation for a philosophical investigation is what I mean by the methodological problem of kinds. In much of philosophy of science, the semantic question is reframed as part of a larger project to provide a responsible descriptive characterization of the apparent success (and failure) of science to develop theories, models, concepts, and explanations. Consider, for instance, the following two examples. First, the account developed in Chang's *Inventing Temperature* [8]. The book traces the evolution of the concept temperature during the revolutions in scientific measurement capabilities of the 18th and 19th centuries. Chang demonstrates how precisifying what was meant by "temperature" and associated terms (e.g. "melting point," "boiling," and, interestingly, "comparability") was an iterative process of meeting conceptual ambiguities with changes in measurement technology and meeting increased measurement capabilities with new conceptual queries. By way of analyzing this historical process, Chang introduces his theory of conceptual extension (pp. 141-158). His theory offers a mechanics of conceptual evolution and refinement that relies on multiple instrumentation techniques agreeing on a value ("mutual grounding," pp. 156–158) as a predominant method of conceptual extension. In this account, the uses of "temperature" and its affiliates are not considered for the sake of semantics, but instead in order to understand how clarifying the referents of such terms aids the development of scientific practices and contributes to the structure of scientific theories. Chang has broadened this conceptual-extension project to include accounts of "acid," [10] "water," [11] and "phlogiston," [9] among other concepts. These projects contain responses to the semantic problem, but they are solutions to the methodological problem: mutual grounding and Chang's accounts of the usage-histories of kind terms are responses to the question of how scientists use kind terms to accomplish their projects.

Second, consider Wilson's account of concepts from Wandering Significance [32]. One of the central positive projects of the book is to articulate a theory of how science influences the development of concepts, and vice versa. Wilson develops an account of scientific theories in which the

³It is worth noting that recent work on kinds in the philosophy of psychiatry, e.g. [27], has addressed just this question of the value of classifying mental disease and symptom categories.

conceptual architecture of a theory is much less cohesive than it might, on first glance, appear. He calls this view the "theory façade" account. In this account, theories are made up of "patches" in which a concept is well-defined over a given domain. Domains are individuated by reference to various uses to which the concept can be put and various parts of the world that the concept reliably picks out (if questions are asked of the concept in the right way). To understand Wilson's account as a response to the methodological problem, it helps to focus on one feature of the ways in which Wilson defines patches, which can be seen most clearly in his discussion of hardness:

Our usage of the predicate "is hard" displays a fine-grained structure that we are unlikely to have noticed, for our everyday usage is built from local patches of evaluation subtly strung together by natural links of prolongation. More specifically, in everyday contexts we adjudicate the "hardnesses" of various materials, both comparatively and absolutely, through a wide variety of comparatively easy to apply tests—we might squeeze the material or indent it with a hammer; attempt to scratch it or rap upon it; and so on. In most cases, we will be scarcely aware of the exact technique we will have employed for this appraisal: "Did I rap, squeeze or scratch that piece of wood? I can't really remember." In fact, our choice of tests is likely to have been suggested by the material in question: we instinctively appraise a wood by rapping upon it, a rubber by squeezing, a metal by attempting to make a small imprint; a glass or ceramic by rapping lightly or scratching (not by trying to make a small imprint!). In fact, we are normally interested in comparing hardnesses mainly within natural groupings of stuffs of generally allied characteristics, generally metals with metals, ceramics with ceramics and so forth, although interesting crossover cases also arise. [32, p. 336, emphasis added]

Wilson goes on to examine the variety of measures for hardness across various material domains, concluding that,

our employment of "hardness" silently distributes itself into a patchwork of sheets, locally distinguished by a certain vein of probing (scratching, tapping, etc.), that sit over various varieties of material stuffs and continue smoothly into one another. . . . As an inferential tool, most of us employ the term "hardness" informally as a generic, single-scale "folk physics" parameter that we consult in selecting a material for, e.g., manufacturing purposes. Left at this general level, the term requires further specialization before it can carry much data usefully. Accordingly, over each localized domain of related stuffs, the "hardness" parameter is likely to silently specialize on the forms of probing that prove most informative with respect to the materials and purposes locally at issue. [32, p. 338]

This discussion suggests that the "patches" that comprise the conceptual structure of scientific

theories often arise as a consequence of the tendency of members of certain higher-level kinds (e.g. metals, as opposed to gold) to exhibit similar properties or behaviors—that metals are all susceptible to scratch tests is both a fact about how the concept hardness behaves around that kind of materials, as well as a fact about the class of materials themselves. To put the point in slightly different terms, the "natural groupings of stuffs of generally allied characteristics" that make up kinds of (at least) scientific interest are kinds because they exhibit shared properties of interest to science. And this interest is not arbitrarily designated: those properties of interest to science are just those that can be robustly detected, measured, manipulated, and intervened upon.⁴ In order to explain how classification aids the practice of science, it becomes necessary to formulate an account of how these groupings of properties manifest, how they are measured, whether they can be controlled, and what explains them. These are the sorts of questions the methodological problem of kinds addresses.

Reconsider the puzzle that began this article in light of the methodological problem. The three cases of gold atoms—the macroscopic lump of gold, the collection of gold nanoclusters, and the collection of gold atoms—exhibit different groups of properties. In fact, the properties of the different cases are so different that it is difficult even to develop a basis of comparison for properties they share: the macroscopic lump is shiny, yellow, malleable, ductile, inert, has a melting point, not to mention certain secondary economic properties, and so forth. On the other hand, the collection of nanoclusters is catalytically active, exhibits an LSPR response, appears as a reddish-brown-hued solution (or, when dried out, as a nondescript dark stain in the bottom of a test tube), and is necessarily locked into relationships with various stabilizing chemicals. Finally, the collection of individual atoms, which is admittedly a wholly theoretical but conceptually useful potential arrangement, exhibits only the properties of individual gold atoms, namely electronic configuration, orbital symmetries, quantity of neutrons and protons, etc. It is not simply that properties such as color change their value (from yellow to brown) in the move from one case to another, but rather that some properties, such as temperature, LSPR response, and orbital symmetry, only exist at certain scales.

I have shown that the methodological problem of kinds, namely the question of how classifi-

⁴In this light, then, the groupings of properties to which Batterman, Butterfield, and others refer in their discussions of "universality classes" are really just a special case of scientific kinds.

cation aids the practice of science, is answered via discussions of the groupings of properties that scientists use to classify, that is, discussions of the measurement, organization, explanatory power and apparent universality of properties across a kind or set of kinds. In this light, the differences in properties among the three cases of gold atoms leads to two distinct conclusions: (1) The three cases are different kinds under the auspices of scientific investigation, and (2) Scale plays a role in delimiting the groupings of properties that demarcate kinds. This means that the methodological problem of kinds requires, as part of its solution, an understanding of the role of scale in classification.

In the remainder of this article, I show how scale influences classification, concentrating on the scientific problem of developing a classification scheme for nanoscale materials. While the role of scale is particularly vivid in nanoscience, my remarks generalize to other areas of scientific enterprise. The reason for this generalizability is itself part of a response to the question of how properties group. In the vast majority of sciences, phenomena, objects, and properties group around characteristic length and time scales, from the vast expanses of time studied by geology to the sub-picometer regions of space studied by particle physics. Scale is a constraint on the manifestation of groupings of properties, and it is also a rationale for observed interactions between phenomena. It is (part of) the reason that things can be grouped together along property lines at all; because many properties are scale-dependent, comparisons of property groups across widely divergent length and time scales are, in a certain sense, incommensurable. At the same time, small things do interact with big things, which means it is necessary to model interactions across a variety of scales. The scale-dependence of properties makes it clear why this task is not straightforward.⁵

The title of this article draws from the common car-trip game 20 Questions, in which one player thinks of an object and other players take turns asking yes-or-no questions (up to 20 in all) to figure out what the object is. Whoever guesses correctly first wins, and if no one gets it, the player who thought of the object wins. One of the most common and most effective starting questions for the game is "Is it smaller than a bread box?" The utility of this question at partitioning the possible objects in a 20-questions game illustrates just how powerful a role scale plays in underwriting classification.⁶

⁵Wimsatt [35, pp. 193–240] has discussed the problem of modeling interactions across length scales in his considerations of compositional levels of organization.

⁶Of course, the bread-box question is only actually effective when one knows about how big a bread box is. For

3 Chemical Kindhood: Reactivity, Microstructure, and the Structure– Property Paradigm

Chemical phenomena exist across multiple characteristic length scales, develop conceptual infrastructure native to each scale, and connect phenomena at one length scale to properties at another length scale. Chemical reactions, for instance, are generally taken to be macroscopic phenomena—the result of pouring the contents of a test tube into a beaker, to caricature—but they are frequently explained in terms of microscopic changes in the molecular structure of the reactants. So it is natural to wonder whether chemical kinds, both infimic kinds such as the individual chemical elements and 'higher-level' kinds such as acids and metals, are microscopic or macroscopic.

The literature within philosophy of chemistry is, unsurprisingly, divided. There are arguments that chemical kinds are microstructural, such as Hendry's [12] and Le Poidevin's [16]. There are arguments that they are macrostructural, such as Needham's [19] and van Brakel's [28]. And there are a host of conciliatory, perspectival, and deflationary approaches, such as Ramsey's [23] contextualism, Weisberg's [30] argument against the coordination between scientific and everyday kinds, VandeWall's anti-essentialist critique of Ellis [29], and LaPorte's [15] essence-discovery model. A recent contribution of the latter sort comes from Bursten [4], who argues that chemical kinds are individuated macroscopically according to a criterion of similarity of chemical reactivity, but that this macroscopic similarity is explained by similarity of microstructural change. In her account, changes in the atomic composition and/or the microstructural arrangement of atoms in a substance or compound are necessary and sufficient conditions for changes in chemical reactivity, but they are distinct from the macroscopic patterns of reactivity that individuate chemical kinds.

Drawing the explanatory connection between microstructure and macroscopic reactivity does ease the tension in the literature, as well as reflecting chemical practice. But it does not in itself explain why chemists need both macroscopic and microstructural ways of conceiving of chemical species. In the remainder of this section, I propose a corrective to Bursten's account, namely that her argument that microstructure is an explanatory basis for chemical reactivity does not go far enough. What is missing was the following: one of the central purposes of classification

those whose childhoods included neither 20 Questions nor bread boxes, perhaps a better partition here would be "Is it smaller than the 10-volume Routledge Encyclopedia of Philosophy?"

in chemistry is to develop explanations of a "scale-bridging" sort—that is, to justify macroscopic changes in reactivity on the basis of microstructural changes. This pattern of reasoning is pervasive in chemistry and essential to chemical practice, and so it is crucial in a methodological account of chemical kinds.

Consider a few examples from a variety of chemical eras and theories of explanation:

- 1. A notable experimental achievement in 18th-century chemistry was the macroscopic detection of fixed airs, which allowed Priestley, the Lavoisiers, Black, et al. to confirm theories, albeit (purportedly) conflicting ones, about the microscopic actions of gaseous principles.
- 2. Dalton's laws of constant and multiple proportions are macroscopically-tested laws usable in hypothetico-deductive explanations of microstructural chemical behavior.
- 3. Kekulé's celebrated discovery of the ring structure of benzene led to a unification 19th-century chemists' understanding of the macroscopically-individuated aromatic compounds via identification of the ring structure common to the compound class.
- 4. Contemporary Periodic Tables of the Elements contain both microstructural and macroscopic information about each chemical species in the table (viz., electronic structure, thermodynamic phase at standard atmospheric temperature and pressure).
- 5. Contemporary textbook representations of organic reaction cycles, such as the Krebs (citric acid) cycle, frequently depict macroscopic interventions, such as the addition or subtraction of water, performed on the central molecules undergoing cellular metabolism.

Each of these examples connects macroscopic and microscopic concepts in chemistry by means of experiment, observation, and control of the manifestation of properties at multiple characteristic length, time, and/or energy scales. This central feature of chemical conceptualizing, then, must be aided by—or at the very least not hindered by—the classification practices of chemists. And chemists themselves have a vocabulary for describing this microstructure–macroscale connection: the *structure–property relationship* or the *structure–property paradigm*. In fact, the bigram "structure–property" appears in over 80,000 scholarly texts published since the year 2000 and indexed in Google Scholar; "natural kind," on the other hand, appears in about 14,000. While it is

rarely defined explicitly, the structure–property relationship is the explanatory connection between microstructure and macroscopic properties that has been identified here, as seen in these excerpts from a variety of subfields in chemistry and engineering:

- 1. "Correlating the material's electronic and macromolecular structure to the observed electrical and optical properties have been difficult due to the lack of structural integrity of the materials under investigation. ... The major problem is that the theories used to explain electrical and optical properties often are based on a single structural type and the measurements are made on structural mixes." [17]
- 2. "The objective of this work was to correlate the molecular-scale structure of surfaces with their ability to resist the adsorption of proteins from buffered aqueous solutions." [21]
- 3. "[A]s the structure becomes simpler, the ferromagnetic ordering reduces indicating the structural dependence of the magnetic ordering." [14]

Additionally, there exist chemical modeling techniques known as quantitative structure—property relationship models, the purpose of which is to develop analyses of structures that correlate with the greater or lesser expression of a given property.

The mandate from the methodological problem of kinds in the previous section encourages philosophical reflection on how classification aids the practice of a science. While deferring to the norms of practice for a science may not always reveal the deep conceptual structure underlying that science, it is a boon to the present account of classification that the structure–property paradigm appears as a conceptual framework and modeling tool in contemporary chemical practice. Further, the structure–property paradigm tacitly assumes some sort of scale-separation between the microstructure and the macroscale property it explains. The "structure" of structure–property relations is never the incidental macroscopic structure of a sample; it is the molecular-geometric or electronic structure of the smallest reproducible units in the substance under consideration, be they molecules, functional groups, unit cells of crystals, individual atoms, or some other microstructural feature of note. "Property," on the other hand, typically refers to a feature produced by collections of structures, such as color (an optical property), heat capacity, ferromagnetism, or electrical conductance.

Chemists work with kinds at a variety of scales, and each of these kinds is a grouping of features, structural or otherwise, of interest to chemists. At the macroscopic scale are chemical species that may be identified and re-identified by their reactive properties (e.g. inertness, solubility in water). At the microstructural scale are molecular geometries, such as the familiar mickey-mouse shape of a water molecule, the double helix of DNA, or the zig-zag chain of carbon atoms in the hydrocarbons that make up fossil fuels and natural gases. At a still smaller scales are the symmetries of atomic electrons, which dictate constraints on the ways in which atoms can combine to form molecules.

One way to understand this scale separation that underlies the structure–property paradigm is to note that each of the characteristic length scales of chemistry houses its own conceptual infrastructure, that is, its own kinds. "Gold" is not a useful kind for articulating the properties of orbital symmetry groups (presence or absence of an inversion point, number of permitted rotations and reflections, etc.), and neither is "point group" for articulating the properties of macroscopic gold (inertness, malleability, non-conductivity, etc.). Taking the archetypical example from the literature, under this framework, "water" and "H₂O" are kinds that index to different length scales, a feature that both explains their non-identity and which indicates the possibility of some other relation—such as the asymmetric explanatory one underlying the structure–property paradigm—bridging the gap between them.

So, instantiating the structure–property paradigm in a theory of chemical kinds requires some tacit acknowledgement of the scale separation between microstructural features of atomic, crystalline, molecular, and other chemical species, on the one hand, and their macroscopic, reactivity-individuated analogues, on the other. Making explicit this scale separation reaffirms the received view in philosophy of chemistry that molecular kinds like "water" are distinct from macroscopic kinds like "H₂O," and it provides the missing pathway for drawing relations between the two sorts of chemical kinds.

However, the waters (or is it H_2Os ?) begin to muddy at the nanoscale. Here the role of scale in individuating chemical kinds is all the more striking, even as scale separation between microstructural and macroscopic features begins to break down. In the next section I argue that to preserve the effectiveness of the structure–property paradigm in nanoscience, one need consider not only chemical composition, but also the size, shape, and surface chemistry of materials under consideration. Only once these features are all specified is it possible to classify nanomaterials

according to differences in properties of interest. This shows that classification of nanomaterials differs from classification in other areas of chemistry as a result of differences in the scale of the materials being classified.

4 Scale-Dependence and Nanoscale Kinds

The nanoparticles described in Section 1 participate in different chemical reactions than macroscale gold, such as their ability to act as catalysts for other reactions. Where bulk samples of gold are known for their non-reactivity, gold nanoparticles can be used to speed up or increase the yield of chemical reactions. For instance, it has recently been shown[37] that small, gas-phase gold nanoparticles can be used to catalyze the oxidation of styrene, the molecule that forms the basis of styrofoam cups. Under the account referenced in the previous section, this makes those nanoparticles a different chemical species than bulk gold. But so are the particles distinct from isolated gold atoms, because the nanoparticles' catalytic effect is a macroscale property.

Nanoscale kinds present a sort of double-edged Sorites paradox: when a sample of a material gets too small or too big, it ceases to be a nanomaterial. But the lines between molecular, nanoscale, and macroscale materials are fuzzy at best. It is common for nanoscientists to speak of molecularly-structured, 13-atom clusters of gold as nanomaterials, while there are many materials five or ten times larger than those clusters that get counted as molecular materials. For nanoscientists, while boundaries of size are an acceptable rough first pass, it is really the scale-dependent properties of nanomaterials that define them as nanomaterials. These properties are the same ones that raise the question of whether it makes sense to treat gold nanoparticles as of the same kind with either atomic or macroscale gold. Extending the structure–property paradigm to nanomaterials, then, requires building up a classification scheme that captures the relevant structural features of nanomaterials that correlate with properties of interest.

Most accounts of chemical kinds, including the one referenced in the previous section, are founded on the idea that composition, that is, elemental makeup, is the foremost grounds for classification in chemistry. For many chemical substances and processes, composition dictates structure, and is thus an essential sortal for chemical properties. The centrality of composition is easily understood by considering the relationship between composition and molecular, as well

as electronic, structure. The microscopic composition of a substance is its atoms, arranged into molecular (covalent or ionic) structures. While composition alone underdetermines the structure of a given compound, it *constrains* structure by limiting the available electronic configurations of an atom, which in turn constrain the number, kind, and arrangement of chemical bonds into which the atom can enter. For both "fundamental" chemical kinds (i.e. individual elements) and higher-level kinds (e.g. metals, noble gases), composition is the primary constraint on structure.

One of the central differences between nanomaterials and chemical materials writ large is that for nanomaterials, composition no longer takes such a center stage. The relevant groups of properties of nanomaterials, and the relevant structures that correlate to those properties, are underdetermined by the specification of composition alone. While specification of non-compositional properties of macroscopic chemicals, such as the phase (solid, liquid, aqueous, gaseous) of a given sample, its temperature, or its quantity is often useful for understanding reaction dynamics, that is, how quickly and through what intermediates a reaction will proceed, specification of its non-compositional physical properties is inessential to the determination of macroscopic chemical kindhood if its microstructural analogue is specified. Macroscopic gold is still gold, whether solid or molten. But at the nanoscale, one needs to know significantly more about the physical properties and chemical environment of a material in order to determine its relevant reactive properties.

The additional information that one needs about nanomaterials can itself be classified into three categories, in addition to composition. These categories are dimensionality or shape, size, and surface chemistry. Dimensionality classifies nanomaterials into 0-, 1-, or 2-dimensional categories, indicating the number of dimensions of the material that extend above the nanoscale. 0-dimensional nanomaterials have no dimensions above the nanoscale; the nanoscale gold spheres in my sample above are 0-dimensional nanomaterials. For 0-dimensional nanomaterials, differences in shape (spherical, cubic, triangular prismatic, etc.) often lead to differences in properties such as LSPR response or chemical stability. 1-dimensional nanomaterials are long wires, tubes, or belts, often used in electronics for their ability to conduct electricity along macroscopic regions in one dimension. 2-dimensional nanomaterials are thin films, used as coatings for other macroscopic materials to protect against bacteria or as components in solar cells.

⁷An alternative means of specifying macroscopic chemical samples is to determine the characteristic phase diagram of a substance or a reaction. I thank an anonymous reviewer for adding this point

Size is a relevant classificatory principle for nanomaterials because small nanomaterials, extending around 2–3 nanometers, behave very differently than large 0-dimensional materials; likewise thickness of a wire or thin film can influence the properties a material is designed to exhibit. For 0-dimensional materials, those under 5 nanometers are often referred to as nanoclusters, and these are closer to molecular materials than larger nanomaterials in the following way: different tokens of the same kind of nanocluster generally have the same molecular geometry as one another, where different tokens of the same kind of larger nanomaterials may vary in molecular geometry. A common nanocluster, for instance, is ${\rm Au}_{13}$, a pseudo-spherical "molecule" of gold atoms with a specific bonding geometry. On the other hand, gold spheres around 50–60 nm in diameter may vary in molecular geometry⁸ and in the number of atoms in a given sphere without varying much in stability or LSPR response.

The role of surface chemistry in constraining the properties and behaviors of nanomaterials, as well as constraining their developing structure, is perhaps the biggest difference between nanomaterials and their macroscopic counterparts. Because nanomaterials are so small, a significant fraction of atoms in any nanomaterial lies on the material's surface. This makes nanomaterials less stable than macroscopic samples of substances or compounds with the same composition, because surface atoms are less stable than interior atoms. In order to stabilize nanomaterials, chemists add additional compounds to the reaction when synthesizing nanomaterials. These additional compounds, called surfactants or capping agents, act like sausage casings to hold together the atoms of a nanomaterial and maintain its shape over time. Some capping agents can only exist in water-based environments; others require organic (oil-like) environments. Different capping agents occlude the surface of the nanomaterial to different degrees, making it more or less difficult for a nanomaterial to react with other materials. The same capping agent can be used across a variety of compositions, but often will constrain the shape materials differently from one composition to the next. The capping agent poly-(vinyl pyrrolidone), for instance, tends to produce cubic particles of silver and branched, tree-like particles of gold.

This exposition of nanoscale classification shows that for nanomaterials, specifying composition—

⁸One way of understanding this difference is by thinking of larger nanomaterials as crystalline, rather than molecular, materials. Larger nanomaterials are often analyzed by electron diffraction for crystallinity, where small nanoclusters are comprised of directed, molecular bonds.

⁹The reason for this relative instability is that surface atoms are bonded to fewer other atoms in a sample than interior atoms, making surface atoms easier to remove or, inversely, more difficult to keep in the same place.

even when composition is supplemented by information about microstructure drawn from the structure–property paradigm—is insufficient to specify kindhood. The tetrad of composition, dimensionality, size, and surface chemistry provides a more useful, though perhaps a dauntingly fine-grained, set of classificatory principles. I will comment on the fineness of grain shortly, arguing that it is endemic to nanoscience as a synthetic science. But before I do, I want to step back and consider how this four-part classification scheme fares with respect to the methodological problem of kindhood I defined in Section 2.

I said earlier that the reason philosophers of science concern themselves with kinds is neither strictly metaphysical nor wholly grounded in concerns about reference; rather, I argued that the motivation for questions about kindhood in philosophy of science stems from a need to develop an account of the role of classification in carrying-out of science. Whether one takes science to be carving nature at its joints or merely developing empirically adequate, usefully projectable, or inferentially reliable categories, classification is a tool used to help develop scientific concepts and determine whether or not a theoretical principle applies to a given situation. So the fact that the classification of nanomaterials differs from the classification of macroscopic materials, as well as from the classification of molecules, implies that the concepts and theories that make sense of matter at the nanoscale are themselves distinct from the concepts and theories that make sense of molecular and macroscopic matter.

While this result is not necessarily surprising in its own right, paying attention to how the interests of classification change across scales can provide insight into the question that arose out of Section 3, namely, how do macroscopic and microscopic classification schemes in chemistry connect to one another? The emphasis on surface chemistry in nanoscale classification is not repeated at either a higher or a lower scale, which suggests that the transition from microscopic to macroscopic phenomena is more conceptually complex than merely aggregating properties of atoms over a large-number sum. Likewise, the appearance of novel phenomena unique to the nanoscale countermands traditional, reductionist accounts of macroscopic properties of substances being explicable entirely in terms of properties of individual atoms. And, rather than urging an about-face from reduction to its philosophical counterpart, emergence, the appearance of novel conceptual and classificatory structures in nanoscience shows how attention to the movement between scales, rather than to a destination at the very big or the very small, can reveal complex conceptual mechanics.

At the nanoscale, the properties and behaviors that stem from the shrinking scale of the material in question become more important than the properties and behaviors that originate from the elemental identity of the material. Another way to frame this point is to say that for gold nanoparticles, the change in the scale of the material serves as a change in properties associated with a change in microstructure. By the structure–property paradigm, this change needs to be reflected in the classification scheme used to categorize nanomaterials. And this change in classification will itself percolate up to changes in the concepts and theories used to describe those materials.

The development of new conceptual infrastructure at the nanoscale is an instance of the scaledependent introduction of new concepts, theories, and models across especially the physical, but likely also the life and human, sciences. Wilson [34] addresses shifts in the conceptual structure of a scientific theory that result from changing theoretical contexts by discussing the interrelations between point-particle, rigid-body, and flexible-body mechanics. While he does not frame his discussion explicitly in terms of scale, one of his central concerns is the ways in which larger-scale systems suppress information about smaller-scale behaviors, a process that requires mathematical approximation techniques and variable reduction and which he calls "physics avoidance." Batterman [2], on the other hand, has emphasized changing scale as a driving force for changes in conceptual structure, sparking an ongoing debate (cf. e.g. [5, 6, 24]) over the essentiality of renormalization-group approximation techniques for developing conceptual understanding of certain physical systems. This debate continues to highlight the fact that many scientific concepts are anchored to particular scales. So the scale-dependence of the classification schemes—and, thus, of the conceptual and theoretical infrastructure—of nanoscience is not unique to the relation between chemistry and nanoscience. Rather, it is simply a particularly evocative instance of a pervasive scale-dependence in contemporary scientific theories.

While the scale-dependent motivation for changing classification schemes is not unique to nanomaterials, there is one difference worth mentioning between the classification of nanomaterials and other scale-dependent developments of novel classification schemes. I mentioned earlier that the tetradic division of structural features of nanomaterials would appear to lead to a particularly finely-wrought taxonomy of nanomaterial kinds, and this is no illusory appearance—a common goal of articles on the synthesis of nanomaterials is to introduce the reader to a supposed new kind of material with new structures and new properties.

Recall that the methodological problem of kinds, which motivates debate about kindhood in philosophy of science, is to determine how classification aids the carrying-out of scientific projects. Given this framework, one can see how differences in the goals of scientific projects can and should lead to different sorts of classification schemes. Classificatory projects in some sciences aim to find a small, finite number of phenomena or objects, such as the 61 particles identified by the Standard Model of Particle Physics or the 92 natural chemical elements in the Periodic Table. Classification schemes of this sort aid the descriptive scientific projects, such as the development of dynamical theories. On the other hand, many scientific projects—including much of chemistry and nearly all of nanoscience—aim to synthesize new substances and materials, and thus to generate new kinds to be added to an open-ended classificatory scheme. Even the projectability of the classificatory principle underlying the Periodic Table (that is, integer increases in nuclear charge) produces an open-ended, though not anarchic, classificatory scheme. On the other hand, traditional biological classification into taxonomic (i.e. 'tree-like') speciation have relatively little to do with synthesis, reinforcing the idea that different sorts of classification schemes are indexed to different scientific purposes.

The tetradic classification scheme of nanoscience, which sorts materials by composition, dimension, shape, and surface chemistry, generates a dense network of possible kinds with a variety of interrelations. One can partition the network into regions by any of the four sortal criteria, or by combinations thereof. This map of structural features identifies not only individual nanomaterial kinds, but similarity of structure among higher-level classes of kinds, allowing for comparisons, e.g., of properties among metal nanowires of different compositions or of differences in optical response between gold nano-spheres of different sizes. These comparisons are not merely hypothetical; they are descriptions of current research projects in synthetic nanoscience laboratories [26, 31, 25, 36].

This classification scheme also indicates to researchers different ways in which an existing particle may be modified to obtain a desired difference in properties of interest to various applications of nanomaterials. The structure–property paradigm indicates that changes in structure correlate to changes in properties, and as research in nanoscience progresses scientists are developing better control over desired properties by refining their ability to manipulate the structure of synthesized materials.

Such projects are rather far-removed from questions aiming to locate the essence of a newly-

synthesized material, and those with heavily naturalist intuitions might worry that the very synthetic nature of such materials belies attributions of essence. And although there is a rather practical worry about consistency of naming of similar particles created by different labs, the question of how reference attaches to newly-synthesized particles is less of a philosophical concern—nearly every new particle architecture is baptized by reference to some or all of the four structural features, e.g. "poly-(vinyl pyrrolidone)-capped silver nano-cubes"—than it is a headache for researchers whose particles lie in a nebulous somewhere between "sphere" and "cube." But in order to manipulate and control the properties of newly-synthesized particles, and in order to understand the relation between those properties and the structures of nanomaterials, the four-part classification scheme is an essential tool. This is the point of classification in nanoscience, and consequently, deconstructing the tetrad is a more productive project for philosophers of science than is arguing for the (lack of) essence of nanoscale kinds or projectability of nanoscale kind terms.

5 Conclusions

In Section 2 of this article I showed that neither metaphysics nor reference are essential to resolving the endemic problem of kinds in philosophy of science. I identified that problem as the one of how classification aids the aims and methods of science. I called this problem the methodological problem of kinds, and I have offered a response to the methodological problem that is specific to chemistry and nanoscience, and which nonetheless explains a recent spate of interest among philosophers of science in the role of scale in concepts and theories in the physical sciences. With the three cases of gold atoms that began this discussion I showed that the identity-determining features of chemical and nanoscientific kinds align with different length scales of interest to different projects within those sciences, and that a scale-dependent account of kindhood both responds to the methodological problem of kinds for these sciences and resolves some existing debates in philosophy of chemistry, as well as tracking contemporary chemical practices such as quantitative structure—property modeling. While the structure—property paradigm and scale-dependence are distinct, they are related, and they are each central to the account of kindhood in chemistry and nanoscience presented here. I have focused on these sciences because of their common synthetic aims, which affect the roles classification play in the carrying-out of scientific activities therein. The extent to which each

feature of the account generalizes to other sciences remains an open question, though recent work on scale-dependence in physics has borne fruit, and the structure–property paradigm has analogues in the worries about the correlation between structure and function found in philosophy of biology and neuroscience.

I showed that in nanoscience, a notion of microstructure that includes dimensionality, shape, and surface chemistry alongside composition is an asset rather than a hindrance to the synthetic goals of that science. This suggests that the classificatory practices of nanoscientists are successfully aiding in the carrying out of that science's projects. However, the account of nanoscientific classification I sketched fails to align with many tacit best-practices assumptions in philosophy of science for how to set up classification systems. In particular, the tetradic, bottom-up classification scheme is not a taxonomy, in which kinds are grouped at successively greater levels of generalization. I argued that this is a problem for philosophical preconceptions about classification, rather than for scientists. As a synthetic science, nanoscience has a rather different set of classificatory needs that typical descriptive sciences. While taxonomy may work for those sciences (and the effectiveness of taxonomy in those sciences is still an open question), it is clear that in nanoscience and other synthetic sciences, greater specificity of structure is well worth the cost of a clean-cut taxonomic framework.

This point may not be surprising, but it is one that has received relatively little philosophical inspection up to this point, largely because synthetic scientific projects themselves are not often the subjects of philosophical analysis. Understanding the considerations of synthetic science, though, can aid in an exposition of the latter point. Consider that in synthetic scientific projects, the aim is to make something new, and very rarely is the target creation blindly constructed; instead, a set of heuristics or design principles guide and constrain the scientist's decisions about what sorts of objects, substances, or materials to employ. Materials are selected for their properties, and they are manipulated by altering their structure, further rationalizing the structure—property paradigm.

I also showed that the role of scale as a sortal for classification has been largely overlooked. By this I do not mean that scientists and philosophers have failed to notice that groups of big things are different than groups of small things; rather, scale has been overlooked as a constraint on what sorts of properties, structures, and objects are useful ones for partitioning up a collection of things of scientific and everyday interest. Scale constrains what kinds of kinds are useful to a

given scientific setting, and it explains why talk of, e.g., differences in numbers of carbon atoms does not make sense when one is trying to determine whether two macroscopic samples of steel are of the same kind.

To clarify, reconsider the three cases of gold atoms that began this essay and consider how each case would be analyzed in a synthetic setting. The macroscopic lump of gold has macroscopic properties, ductility and malleability, as well as chemical inertness, that are similar to other noble metals (e.g. palladium and platinum), as well as to many plastics. The gold atoms, on the other hand, have electronic symmetry, namely d10s1, that is shared by copper and silver. The nearby kinds in the macroscopic case are different than the nearby kinds in the microscopic case; scale has dictated a difference in the kinds of kinds that are relevant in each setting.

As for the gold nanoparticles, it should now be clear that they were themselves underspecified in the original example—their surface chemistry, shape, and size is indeterminate from the introductory description. But knowing that these are the features of the nanoparticles that need to specified to generate relevant alternatives still illustrates the point, which is that classification in the sciences depends on scale and scientific intent, and the properties that aid synthetic scientists in selecting among a range of materials vary with the scale of the system being studied.

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