




# Classifying and characterizing active materials

Julia R. S. Bursten<sup>1</sup> 

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## Abstract

This article examines the distinction between active matter and active materials, and it offers foundational remarks toward a system of classification for active materials. Active matter is typically identified as matter that exhibits two characteristic features: self-propelling parts, and coherent dynamical activity among the parts. These features are exhibited across a wide range of organic and inorganic materials, and they are jointly sufficient for classifying matter as active. Recently, the term “active materials” has entered scientific use as a complement, supplement, and extension of “active matter.” At the same time, new work in the philosophy of science has considered the problem of how to classify the products of synthetic and laboratory processes, and the extent to which the aims of classifying natural kinds compare and contrasts with the aims of classifying these synthetic kinds. In this article, I apply those considerations to the problems of classifying and characterizing active materials. In doing so, I also argue for a conception of active materials’ coherent dynamical activity as multiscale, rather than emergent, and I discuss how the special non-equilibrium status of active materials factors in to classificatory concerns.

**Keywords** Active materials · Classification · Multi-scale modeling · Smart materials · Natural kinds

## 1 Introduction

The principal subject of this discussion is the classification and characterization of active materials. By “active materials” I mean engineered materials that employ principles of active matter in their design. Active matter, in turn, is an umbrella term used to refer to systems whose components are self-propelled and thus out of thermal equilibrium, and which often, as a consequence, are able to generate collective, directed action like flocking and swarming. The movement of a flock of birds is often given as

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✉ Julia R. S. Bursten  
jrbursten@uky.edu

<sup>1</sup> Department of Philosophy, University of Kentucky, 1415 Patterson Office Tower, Lexington, KY 40506, USA

an example of active matter, and there are numerous biological systems that exhibit self-propelling and collective, directed action, such as microtubules and actin microfilaments. Scientific interest in active materials derives from the desire to mimic these properties of active matter in engineered systems, some organic and others inorganic. One of the aims of this article is to articulate the relationship between three aspects of active materials: (a) the out-of-equilibrium response, (b) the composition of active materials from self-propelled parts, and (c) the collective, directed action characteristic of active-material systems. Achieving this aim will afford the groundwork for the account I then outline, which characterizes active materials as synthetic kinds that exhibit a sustained, multi-scale non-equilibrium response.

To characterize active materials as synthetic kinds may not be particularly controversial, scientifically, but it is of some philosophical interest. Most philosophical work on classification comes from the study of so-called “natural kinds.” Philosophical investigations of synthetic kinds are comparatively few and far between. A recent spate of philosophical work on classification in synthetic biology and nanoscience is the exception that proves the rule. I will show that bringing discussions of active materials into dialogue with this work on synthetic kinds in synthetic biology and nanoscience extends and critiques existing philosophical accounts of synthetic kinds. In order to characterize active materials as synthetic kinds, I build on my previous discussion of synthetic kinds as “products of a targeted search for groups of properties that do not regularly group together” (Bursten 2019, p. 3). This definition of synthetic kinds distinguishes synthetic kinds from just any product of chemical synthesis, which I discuss more below in Sect. 3.

To characterize the non-equilibrium response of active materials as inherently multi-scale is perhaps a less obvious or intuitive move; it, likewise, comes with philosophical consequences. The collective, directed action of active materials is sometimes analyzed as an example of emergent behavior, and this analysis imports more than a century of philosophical hand-wringing about the relationships between parts and wholes and among various scientific theories. Recent philosophical interest in multi-scale modeling has led some contemporary philosophers of science to re-examine the premise of the phenomenon of emergent behavior and seek alternative frameworks for understanding relationships among the parts of systems and the theories and models that describe those relationships. For instance, Batterman (2001, 2003) has advanced an account of universality as an alternative to emergence, which produces a novel analysis of what constitutes a satisfying explanation of observed collective behavior. More recently, Batterman (2012), Batterman and Rice (2014), Bokulich (2018) and Green and Batterman (2017) have applied this analysis to multi-scale systems and investigated how varying a modeling strategy from bottom-up to top-down to middle-out changes the explanation of the system’s behavior. In the case of active materials, I will use these recent analyses to advocate for explaining and modeling active materials systems as multi-scale rather than emergent. This argument will reinforce and extend lessons from another article in this issue (Batterman and Green 2020), which uses case studies in modeling steel and bone systems to emphasize the importance of “middle-out” approaches to multi-scale modeling, as well as offering a piece of actionable advice for a scientific audience.

Before moving forward, two prefatory remarks on the scope and intent of this discussion will be clarifying. First, it should be noted that this article is written for a mixed audience of philosophers and scientists. As such, there are times when I will paint with a broad brush both philosophically and scientifically. It is my hope that covering the landscape in this mode will enable more fruitful interdisciplinary conversations about the proper characterization of active materials, which I take to be a subject that belongs neither entirely to philosophy nor to science. In philosophy it is common to speak of work such as this as clarifying the conceptual foundations of a scientific enterprise, and I believe this to be an apt characterization of my present aims. However, unlike many “foundational” projects in philosophy, the goal here is not to create a decision-tree procedure for classifying and characterizing active materials, either through axiomatic or taxonomic approaches. Instead, by defending the view that active materials are both synthetic kinds and inherently multiscale, I intend to leave open the doors for a variety of more targeted classification projects.

Leaving the doors open in this way affords a specific benefit when it comes to the applicability of this research to contemporary scientific practice. Increasingly in contemporary science, data-science ontologies are the preferred mechanism for organizing information about the classification and characterization of synthetic materials. Data-science ontologies (not to be confused with philosophical ontologies) are software systems that can be used to classify materials via building a formal semantic structure within a universe of discourse. Examples include eNanoMapper (<http://www.enanomapper.net/>), The Synthetic Biology Open Language (<https://sbofstandard.org/>), Chemical Entities of Biological Interest (<https://www.ebi.ac.uk/chebi/init.do>), The Materials Project (<https://materialsproject.org/>), and the Open Biological and Biomedical Ontology Foundry (<http://www.obofoundry.org/>). The scientific use of ontologies to manage classificatory data in nearby areas suggests that data-science ontologies will be the mainstream way forward in developing classification practices for active materials. The foundational work in this discussion is intended to be a useful guide in the shaping of future active materials ontologies.

Second, and relatedly, I discuss both the classification and the characterization of active materials in what follows. “Classification,” as I use the term here, refers to the placing of a sample type or token within a principled semantic structure, such as an ontology or taxonomy, on the basis of the sample’s properties, qualities, behaviors, or characteristics. “Characterization” refers to the determination of those properties, qualities, etc., both at the level of identifying the properties possessed by a sample and at the level of identifying what properties are relevant to specifying kindhood in a given domain. For instance, one might *classify* apples according to color, by sorting apple cultivars into red and yellow and green. Within that classification system, one might *characterize* a Granny Smith apple as a green variety. Of course, sometimes Granny Smiths might appear more yellow, or even reddish in spots. Reflecting upon this, one might determine that color is not an important *characteristic* of apple cultivars, and consequently abandon the color-based apple cultivar *classification* project.<sup>1</sup> When it comes to philosophical discussion of kinds, classification and characterization are two

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<sup>1</sup> Systems that classify would-be kinds on the basis of color, such as John Stuart Mill’s white things, are famously likely to end up in the rubbish-bin of philosophy. At least these apples may compost!

sides of one coin. The two become even more intertwined when the kinds in question are not already well-established, that is, when they are instead constructed through scientific and engineering enterprises, rather than plucked as-is out of the world. I will indicate reasons for this connection when I discuss synthetic kinds more generally below.<sup>2</sup>

Below, I develop some foundations for classifying and characterizing active materials. I proceed as follows. In Sect. 2, I discuss current research in active matter and active materials and offer a means of distinguishing the former from the latter. I argue that while active materials research always employs active-matter principles, not all active matter counts as an active material. I suggest that the term “active material” should be applied to synthetic materials with active processes, and I argue that this makes active materials a particular type of synthetic kind. In Sect. 3, I give a brief overview of philosophical concerns related to classification, emphasizing recent interest in the special challenges posed by synthetic, as opposed to natural, kinds. I argue that classification practices from philosophical research on synthetic kinds should be used to develop active materials classification. In Sect. 4, I discuss a microscale and a macroscale dimension of classification for active materials—composition from self-propelled particles and the production of material-wide coherent dynamical activity, respectively. I use the relation between these dimensions of classification to argue that active materials are inherently multiscale, and that it is preferable to conceive of active materials as multiscale rather than emergent for at least some classificatory purposes. In Sect. 5, I consider an additional defining feature of active matter and active materials, namely their status as non-equilibrium systems. I show that the particular way in which active materials are non-equilibrium can be used to distinguish active materials from a nearby class of multiscale synthetic kinds, the smart or response materials. Section 6 contains brief concluding remarks.

## 2 Active matter and active materials

The current scientific literature has not reached a consensus on how to classify types of active materials, which is one of the motivations for the present discussion. However, a reasonable working definition of active *matter* is generally agreed upon: active matter is matter composed of self-propelled parts that generate a collective, directed response. Active matter is related to, but distinct from, active materials. In this section, I discuss the relation between active matter and active materials in order to highlight what qualities of active materials should be emphasized in the construction of classification and characterization schemes for active materials.

The term “active matter” has been applied to a wide range of naturally-occurring and synthetic or engineered materials, as well as to clusters of organic bodies that

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<sup>2</sup> For complementary philosophical perspectives on how to understand the activities of grouping things into kinds, I recommend both Kendig’s (2015) work on “kind-ing” and Havstad’s (2020) recently-introduced distinction between characterization, individuation, and organization as activities of classification. There is an obvious semantic disagreement between Havstad’s distinction and my own (I distinguish classification from characterization, while she identifies characterization as a type of classification), but despite this, I believe our views have more in common than not.

are not typically thought of as materials, such as schools of fish or flocks of birds. The use of “active” in describing active matter can be interpreted in two distinct, though related, ways. First, “active” may be understood to refer to a particular ability of certain types of matter to perform mechanical work or to otherwise direct energy within the system (e.g. by converting energy of one type into another type). Second, “active” may be understood as a description of characteristic behaviors of components of matter: active matter is matter with active parts, understood in contrast to passive parts. These two “actives” of active matter are related by the fact that, in active matter, the first type of “active” behavior is achieved through the second type: the activity of individual components generates collective, directed action that converts energy or performs work.

Both these types of activity in active matter are possible only when an active-matter system is out of thermodynamic equilibrium. Systems out of thermodynamic equilibrium are ones in which energy flows into or out of the system, and ones which, consequently, are capable of macroscopic change. Energy flow into an active-matter system is necessary for the active parts of the system to engage in activity. To conceptualize this difference in biological terms, consider the difference between a flock of starlings resting on a power line and a flock of the same birds flapping in the air. The former is not an example of an active-matter system, as the birds at rest are not doing anything to sustain a dynamic flocking shape or pattern. The flock is “in equilibrium” and unchanging. By contrast, the flights of the individual birds in a starling flock feed a dynamic flocking pattern that can only persist by continued energetic input from the flapping of individual starlings’ sets of wings.

A common model material for active-matter research is the spindle apparatus in cell biology. The spindle apparatus is responsible for the separation of chromatids during cell division. It is primarily composed of a type of polymerized protein structure known as a microtubule, which is found in the cytoskeleton of both eukaryotic and prokaryotic cells. Microtubules are also responsible for cell locomotion, and individual microtubules remain assembled for periods of a few minutes to a few hours. Microtubules assemble and disassemble as the two component proteins in microtubules,  $\alpha$ -tubulin and  $\beta$ -tubulin, attach and detach from their respective ends of the microtubule. This assembly and disassembly, sometimes called “treadmilling,” (Prost et al. 2015, p. 111) drives many of the active behaviors of microtubules. It is how microtubules remain constantly out of equilibrium, and it is also partially responsible for the self-propelling behavior of microtubules in the spindle apparatus. When microtubules form a spindle, they align in such a way that their individual activities impose a collective force on the pair of chromatids in a dividing cell. At this point, the individual activities of microtubules become a behavior of the active matter of the spindle.

In recent years, the term “active materials” has sprung up as an alternative, supplement, or addition to “active matter.” Indeed, in the series of workshops that led to this special issue, participants debated whether the proper name of the sponsoring institute should be the “Georgetown Active Matter Project,” or the “Georgetown Active Materials Project.” I believe there is a principled difference underlying the distinction between active matter and active materials. The difference rests on whether the object of study is principally being studied as a synthetic material designed for the targeted

manipulation of its active behaviors. If so, the object is an active material. If not, the object is a research object used for the investigation of active matter. Importantly, this distinction captures the intuition that, while flocking and swarming behaviors can be used to understand active principles in engineered materials, a flock of starlings darkening the sky is not, in any literal sense, a material.

To reiterate: active materials are engineered or synthetic materials designed to manipulate the active principles or behaviors found in active matter. Defining the contrast between active matter and active materials in this way rationalizes an intuitive resistance to calling biological flocks and swarms “materials.” It also helps to make sense of divergent research streams within active-matter and active-materials research. Active-matter research aims primarily to model, explain, describe, and understand the active behaviors within naturally-occurring or engineered active systems, including simulated systems. Active-materials research aims to apply the principles of active matter—directed action through self-propulsion of parts—to the design of materials.

For instance, consider recent research on active gels. Active gels are composed of cross-linked polymers of cytoskeletal material such as the microtubules described above. In both naturally-occurring and synthetic cytoskeletal gel assemblies, these polymer structures include smaller proteins called “molecular motors” that interact biologically with microtubules and other filament proteins. Molecular motors move around on filaments and can drag or move pieces of filament with them. This combines with the treadmilling effect described above to produce gel structures capable of self-propulsion. In living cells, this process underlies much of cellular locomotion and the physical movement involved in mitosis, and so is a subject of significant biophysical interest. In order to study these dynamics, the cytoskeletal component of cells is isolated and a model material is formed; these are active gels. Some research aims to discover the dynamics of active gels for the purpose of understanding the hydrodynamics of cells (e.g. Prost et al. 2015), while other research aims to create new materials from the active-gel system (e.g. Guillamat et al. 2018). According to the distinction I am proposing here, the former would be considered research on active matter, while the latter would be considered research on active materials.

Distinguishing active materials from active matter in this way emphasizes the synthetic nature of active materials while leaving room for research on active matter to be on either engineered or natural (i.e., pre-existing) active systems. This facilitates the suggestion I make below, which is that the classification of active materials requires conceiving of active materials as synthetic kinds. While the classification of synthetic kinds—stem cells, synthetic biological parts, novel chemical compounds, nanomaterials, engineered materials, and so forth—has been a subject of some recent philosophical interest, most philosophical discussion of classification has emphasized the puzzles and challenges in classifying natural, rather than synthetic, kinds. In the next section, I provide an overview of this research and examine what advantages are afforded by conceiving of active materials as synthetic kinds.

### 3 Synthetic kinds

“Natural kinds” is the term of art in philosophy used to describe categories afforded to us by the machinations of nature; things like gold and methane, lemons and tigers, quarks and quasars. There is significant disagreement among philosophers about whether natural kinds exist at all or whether they are merely products of human desires to make sense of the raw mess around us. How one cleaves onto one side or another of that disagreement bears on one’s philosophical views on diverse philosophical topics across logic, metaphysics, philosophy of language, and philosophy of science. As an example, consider the position that there are no natural kinds, and that instead the categories we assign to objects of scientific investigation are merely assemblages of properties and functions that are convenient to human scientists with their limited and vision-biased perceptive faculties. If science were carried out by dolphins or oak trees or extra-terrestrials, the categories used to express relations among natural phenomena would likely differ. Such a view constrains the possible answers one can give to the question of what the aim of science is: if science is not about detecting “the real” categories of nature, its aim must be something other than amassing records of “the real” categories and how they interact in laws of nature. Conversely, if there are genuine natural kinds, what makes these kinds the kinds that they are, and how can scientists know that the experimental methods they employ are connected to kinds in the appropriate ways?

Interestingly, given the rich history of philosophical consideration on natural kinds, comparatively little has been said about kinds that are explicitly non-natural but which are nonetheless products of scientific experiment and objects of scientific investigation. In my introduction to a recent collection of essays, I defined kinds of this sort as “synthetic kinds” or “unnatural kinds” (Bursten 2019), in an effort to distinguish kinds that are dreamt up in scientists’ notebooks and cooked up in laboratories from kinds that are found in rocks and rivers.<sup>3</sup> The collection investigates nanomaterials and the products of synthetic biology as archetypal examples of synthetic kinds. In the introduction, I argued that the problem of how to classify the products of synthetic and laboratory processes is importantly distinct from the problem of classifying natural kinds. This difference lies in the intention behind creating a synthetic kind, which is to bring groups of properties together in new ways—typically with some sort of potential application in mind—and this difference in intention generates new questions for philosophers of science studying classification, as well as turning down the volume on certain common questions about natural kinds. Here, I aim to adapt and extend this approach to classification as a framework for understanding classification worries in active materials research. In order to accomplish this goal, I will say a few words about what distinguishes the synthetic-kinds approach from other contemporary approaches to scientific classification and why I believe it fits the needs for active materials research in a way that other approaches do not.

While my emphasis on the contrast between synthetic and natural kinds is new, my investigation of laboratory-created scientific kinds is one part in a growing body of

<sup>3</sup> In this view, the term “synthetic” can be understood to refer both to novel kinds of objects created by scientific practices and to the categories developed to classify those objects. I thank an anonymous reviewer for pointing to this potential source of confusion.



philosophical study on the role of classification in scientific practice. Indeed, Kendig (2015) recently edited a volume of essays on this very subject, and philosophers writing across the spectrum of sciences, including Chang (2012a) on acidity, Fagan (2013) on stem cells, Pradeu et al. (2016) on viruses, and Tabb (2019) on psychiatric disorders have all developed arguments about classification by emphasizing the role of scientific activity in the construction of kinds relevant to scientific practice.<sup>4</sup> For instance, Kendig's (2015) own account of classification hinges on re-conceiving classification as not the production of kinds, but the "activity of kinding," referring to the integrated theoretical, modeling, and laboratory practices that enable scientists to identify and characterize the kinds of kinds that they create. Likewise, Chang's meditations on the concepts of temperature (2004), water (Chang 2012b), and acidity (Chang 2012a) all advance a pluralistic conception of the kinds relevant to science by emphasizing the contingent histories, wide variety of experimentally-accessible properties, and theoretical and practical scientific and non-scientific activities that contribute to identifying a subject of scientific investigation as a member of the kind "acid," "chemical compound," or so on.

I am generally sympathetic to these more practice-driven approaches, and I believe the synthetic kinds account is best interpreted as an extension of such views. However, the synthetic-kind account affords some additional infrastructure for interpreting scientific practices around the investigation of specifically synthetic kinds. This is an advantage over the accounts mentioned above. Synthetic kinds are the targets of investigation in a specific set of scientific practices, which begin with the identification of certain advantageous or curious properties of a system and the thought, "Can I generate the same, or very similar, properties in a system that is different from this one?" In other words, synthetic kinds arise from a desire to extend, recombine, extrapolate, or otherwise reach beyond the current landscape of available categories.

This origin affects the way that scientists conceive of synthetic kinds, as well as affecting the prospects for building taxonomic or other organizational systems around such kinds. To illustrate this difference, consider the distinction between the canonical natural kinds of chemistry, the chemical elements, and an archetypal class of synthetic chemical kinds, synthetic polymers (nylons, plastics, and so forth). There is a single property, atomic number, which determines the order in which a chemical element appears in a periodic sequence. There is some disagreement about the proper layout of the full periodic table,<sup>5</sup> but it is largely academic and aimed at questions of how one might best capture the complex metaphysical and epistemic interrelationships between atomic number and other properties of chemical and physical interest, such as atomic weight, isotopic variation, ionization, electronegativity, metallic character, and so forth.

By contrast, there is no single taxonomical or classification system for synthetic polymers. There are classification schemes that group polymers by thermal response (i.e., thermoplastics versus thermosets versus elastomers), schemes that classify polymers by polymeric structure (i.e. linear versus branched versus cross-linked), and

<sup>4</sup> A canonical early example of this practice-driven approach to articulating an account of scientific classification is found in Hacking's (1991, 1993) work on the subject, which draws a distinction between scientific and non-scientific kinds instead of between natural and non-natural kinds.

<sup>5</sup> For a detailed discussion, see Scerri (2019).



schemes that classify polymers by the synthetic route taken to create the polymer (i.e. addition versus condensation). Other, more specialized classification systems based on monomer identity, relation to natural products, or physical properties also exist. These classification systems cross-cut each other, that is, one set of categories does not nest into another.<sup>6</sup> Further, which classification schemes(s) is/are used to identify or characterize a given polymer depends strongly on the experimental or theoretical setting and bears on the design of experiments and synthetic protocols in both research and industrial settings.

Like the Periodic Table of Elements, these polymer classification schemes group each type of polymers based on sets of relations between the structure of a polymer and some set of properties that correlate with that structure; unlike the Periodic Table, however, these synthetic classification schemes do not aim at a single, unified mode of description nor at a taxonomy. For the synthesis of new kinds, there is a strict advantage to this disunity: scientists aiming to synthesize a new polymer, or devise a new synthetic route to a known polymer, can manipulate properties identified by one classification scheme while remaining agnostic about the properties in other classification schemes. Taxonomic systems like the Periodic Table leave very little room for such agnosticism. Relatedly, an implication of these multiple and disunified classification schemes is that the complete set of properties comprising a kind are not going to be captured by description along any one dimension of classification. This provides room for classification and characterization to accommodate new and unanticipated properties that may come to be seen as important in the construction of a synthetic kind, even ones that are not presently identified any current classification system.

The tendency toward disunity in synthetic classification systems generates an important philosophical implication of the synthetic kinds account. Many accounts of natural kinds in philosophy seek the essence of a kind, the thing that explains or underwrites the connection between a kind and its properties. While it is possible to hold that kinds have essences, but not ones that can be captured by a single classification system, it is more common to expect that if a kind has an essence, that essence is in some sense responsible for all the other properties exhibited by the kind, and so that essence should be the used as the basis for classification systems. Again, the Periodic Table provides a canonical illustration: atomic number is (i) generally considered to be the thing that makes an element the kind of element that it is, as opposed to any other, and (ii) used as the principal basis of classification of the chemical elements, and (iii) appealed to in many explanations of chemical and physical properties of both individual elements and element groups. By contrast, the multiple and disunified schemes used for classifying and characterizing synthetic kinds suggest that such kinds are unlikely to have unified essences that will form the basis of classificatory systems and scientific explanations. This is a strong stance on the question of kind essences in its own right, and it also

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<sup>6</sup> Classificatory cross-cutting occurs when a given category is neither a subset nor a superset of two sibling categories. For instance, “quadruped” cross-cuts “mammal” and “reptile,” because some but not all mammals are quadrupeds, and some but not all reptiles are quadrupeds, and mammals are not a subset of reptiles nor vice versa.

indicates that synthetic kinds are unlikely to yield to microessentialist<sup>7</sup> approaches to classification.

There are further philosophical implications of the synthetic kinds account, but they are beyond the scope of this discussion. For present purposes, I have been introducing the notion of a synthetic kind primarily in order to apply this designation to active materials. While some types of active *matter* are naturally occurring and not obviously synthetic, a central aim of research in active *materials* is to engineer chemical and biological materials that emulate properties of active matter in new or reimagined domains. This produces new kinds of materials. The properties of such materials are sometimes described in terms of the biomimetic activity of their components, but the materials themselves are clearly synthetic. For instance, materials described in highly-cited active materials research include:

- Active gels composed of biologically-derived microtubules impregnated with a kinesin-related protein (XCTK2) that acts as a molecular motor (Fürthauer et al. 2019).
- Active artificial membranes composed of giant unilamellar vesicles with photo-sensitive bacteriorhodopsin pumps (El Alaoui Faris et al. 2009).
- Catalytic nanomotors composed of half-gold, half-platinum cylinders that move autonomously in an aqueous hydrogen peroxide solution, due to oxidation reactions between peroxide and platinum (Paxton et al. 2004).

As I have previously argued (Bursten 2019, pp. 2–3), not all products of synthesis are synthetic kinds. Chemical synthesis can, and often does, aim to reproduce natural kinds, either via synthetic routes that imitate naturally-occurring processes or by novel chemical manipulations. In either case, the product of synthesis may be said to be synthetic, but not a synthetic kind of the sort under consideration here. I raise this point in order to note that each of the active materials identified above, and indeed a significant majority of the materials considered in contemporary active materials research, are not merely synthetic materials; they are synthetic kinds. Adding XCTK2 to a pool of microtubules or bacteriorhodopsin to a vesicle accomplishes the synthetic-kind aim of reaching beyond the current landscape of kinds through novel combination. The third, chemical example above is even more striking as a synthetic kind, due to the complex synthetic process required to produce nanoscale cylinders comprised of two metals, commonly known as Janus particles (Jiang et al. 2010).

This discussion has served to establish that active materials are synthetic kinds. A direct consequence of this designation is that, due to the nature of synthetic kinds, researchers in active materials should not expect to generate a unified classification scheme for active materials. Instead, given what has been said about synthetic kinds so far, researchers should expect active materials to be subject to a variety of cross-cutting, partial, and context-sensitive classification schemata. This expectation seems to bear out in the way review articles categorize research about active materials, such as

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<sup>7</sup> Microessentialist approaches to classification attempt to locate the essences of kinds in some microstructural feature of the kind. Yet again, the Periodic Table offers a useful example: a microessentialist will not only claim that the chemical elements have essences (essentialism) but also that the essences of the elements are the number of protons in their nuclei (a microstructural feature that is used as a principle of classification). This approach to kind identification was popularized in the 20th century, largely by Saul Kripke and Hilary Putnam.

in Needleman and Dogic (2017), which classifies active materials research in a variety of ways, including by type of activity (e.g. contractile versus extensile versus nematic motion in active gels), by the biological material from which the active material derives (e.g. cytoplasmic versus full-cell versus subcellular membrane), by scale and density-in-the-material of the active component, and by chemical structure. This contrasts with reviews of active matter, which propose taxonomic classification schemes (e.g. Marchetti et al. 2013). Conceiving of active materials as synthetic kinds rationalizes this apparent messiness by showing that this is not simply confusion or in-progress messiness on the way to a clear and unified taxonomy of active materials; instead, like polymers and like many other engineered materials, a proliferation of partial and cross-cutting classification systems is all researchers can and should expect from the classification of active materials.

Although synthetic kinds resist a unified or taxonomic classification system, there are some general features common to classification schemes for synthetic kinds. Centrally, synthetic classification schemes aim to support the goals of synthetic scientific research, namely to produce and tune new groupings of properties and study the effects—intended and unintended—of combining properties in novel ways. Consequently, synthetic classification schemes are often phenomenological, grouping kinds in ways that support the creation and analysis of a particular type of observed or desired property or behavior. Likewise, a ubiquitous problem in synthetic science is the identification of the factors relevant to the control of desired properties. This problem poses (at least) two further challenges: first, the challenge of how to identify correlations among groups of properties, and second, the challenge of how to identify what the relevant properties are in the first place. The pervasiveness of these challenges offers some insight into why classification schemes for synthetic kinds are expected to be partial and context-sensitive.

Active materials present a somewhat unusual case study in this vein, because the concept of an active material is predicated on a set of behaviors expected of the material's components. For the other classes of synthetic kinds considered in this section, membership in the kind is conferred by structural features of the materials' components: polymers are composed of chained monomer units; nanomaterials are composed of chemical parts confined to a particular spatial scale; objects in synthetic biology are composed of biologically-derived parts arranged in un-biological ways. For active materials, the structure of the components is secondary to the behavior of the components: self-propelling parts embed in a medium that affords the energetic impulse (or, equivalently, out-of-equilibrium status) necessary to generate directed action. In the next section, I consider the role of self-propelling parts, out-of-equilibrium status, and directed action in both the classification and the characterization of active materials.

#### **4 Characterization and classification of active materials as multi-scale synthetic kinds**

Given that active materials are synthetic kinds, it follows that researchers should expect to use multiple, partial, cross-cutting schemes to classify them. This is not, however, to say that there are no principled means of assessing or comparing classification

schemes, or of employing more than one principle of classification at a time. Some schemes will be more useful than others in a given context, and one of the hallmarks of classification of synthetic kinds is the selection, by researchers, of the appropriate dimensions of classification for a given research setting. In polymers, for instance, classification by chemical composition is more useful in research on biocompatibility, whereas classification by thermal response is more useful in materials engineering.

As identified above, a few different ways of classifying active materials have emerged from contemporary research, including by type of activity, by biological origin, by scale, and by chemical structure. These schemes cross-cut each other, and a given active material might be identified within any or all of them. In this section, I discuss a few dimensions of classification for active materials: classification by self-propelled part and classification by dynamical activity. I show that these two classification schemes may be applied to the same active material, and when they are used jointly on a single material, they produce a further system of constraints on the way that researchers model the material. I use this result to argue that active materials should be conceived of as inherently multi-scale kinds.

I begin with self-propelled particles (SPPs). What I have in mind with this classification scheme is the categorization of active materials by the individual-level and population-level properties of a material's dynamic microstructural components. These are the analogues of the individual birds in a flock. There are quite a few kinds of SPPs in active materials research, and one of the goals of designing new active materials is the construction of non-biologically-derived self-propelled particles.<sup>8</sup> For instance, researchers have designed a variety of Janus-structured nanoparticles<sup>8</sup> and placed them in environments that produce catalytic reactions with one of the component metals, but not the other (Kline et al. 2005). This produces directed motion, although whether this can generate collective motion of the type required for active materials is still somewhat uncertain.

Determining what counts as the SPP in an active material is not always trivial. Particularly in the case of active materials derived from cytoskeletal assemblies, there are a few candidates, and a few kinds of candidates, that might be considered the SPP. Above, I described both microtubules and the myosin molecular motors found in active gels. Both these components are microstructural and active, and microtubules can engage in activity either through the action of molecular motors or through independent assembly and disassembly. There are other types of filament proteins and molecular motors with similar patterns of interaction.

If one were observing this array of microstructural parts and interactions from the lens of natural kinds, this complexity and heterogeneity would be a problem to solve in order to develop a taxonomy of SPPs. Instead, under the framework of synthetic kinds, it is merely a feature of the ataxonomic structure of classification of active materials by SPP type. Moreover, since the synthetic-kinds account counsels a contextual approach to classification, the existence of multiple candidate SPPs in active gels suggests that other aspects of classification and characterization might constrain which SPP to identify as the relevant one for a given research endeavor. Scientific practice appears

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<sup>8</sup> That is, nanoparticles where one spatial half of a particle is composed of one metal and the other half is composed of another metal.

to bear out this suggestion, as there is active-materials research on the activity of microtubule assembly and disassembly, on the contractile action of myosin, and on the transduction-type interactions between microtubules and myosin, as well as analogous studies on other SPPs derived from the cytoskeletal system.

Next, I consider dynamical activity. One of the central requirements for characterizing either a sample of active matter, or an active material, is to develop a model of the collective dynamical activity that it exhibits. There are many such models. Some treat the matter or material as continuous, such as the topological-defect model of active gels developed by Kruse et al. (2004). Other models construct descriptions of the dynamics of collective motion from the dynamics of particulate bodies, such as the Vicsek model of swarming (Vicsek et al. 1995). Some phenomena associated with collective motion are shared among both continuum and particulate models of collective motion, such as the phenomenon of a phase transition that indicates a change in dynamical description once a certain energetic or population-density threshold has been achieved. Other phenomena are applicable only to continuum models of collective motion (e.g. the elastic modulus described in the Kruse model), or only to particulate ones (e.g. the requirement of alignment between particulate “agents” and their nearest neighbors in the Vicsek model).

For many active-material systems, it is possible to model dynamical activity with either a continuum or a particulate model; however, it is not possible to model dynamical activity with any continuum, or any particulate, dynamical model. For instance, the Kruse model describes the conditions required to develop a variety of types of collective motion, such as swarming, the formation of vortices, the formation of asters, and the formation of swirls, in active materials (Kruse et al. 2004). At least some of these varieties of collective motion can also be modeled by extensions of the Vicsek model (Chaté et al. 2008). The type of dynamical structure formed by collective motion in an active material—swarming, swirling, aster formation, contraction, the formation of a polar or a nematic phase, and so on—is a classification basis for active materials, and it is one that cross-cuts the choice of whether to model the material with continuum or particulate models of the material’s collective motion.

I bring this up in order to point out that the selection of a particular dynamical model may assist in characterization more than classification, since in at least some cases the same classification of collective dynamics may be modeled by either a continuum or a particulate model. The appropriate selection and application of modeling schemes to active matter and active materials are a common theme throughout this special issue. While appropriate model selection will not in general advance classification, unpacking some of the subtleties of the approach to classification I advance here may provide additional insight into some of the claims about modeling made elsewhere in this special issue.

I consider two of those subtleties now. Both have to do with the fact that the relevant structures, behaviors, and dynamics of active materials exist at multiple characteristic length scales. First, I mentioned in the discussion of SPPs above that active materials might be classified by both individual type of SPP and population-level properties of SPP, such as the density of SPPs in the active material or the orientation of SPPs relative to one another. These latter features characterize the active-material system at a different scale than the characterization obtained by specifying individual SPP

structures. Following suggestions made elsewhere in this issue, particularly by Batterman and Green (2020), I believe it is productive to recognize these characteristics of active materials as mesoscale characteristics, in contrast to the microscale of individual SPPs and the macroscale of system-wide dynamical activity. Properties of collections of SPPs constrain macroscale dynamics by appearing as parameters in dynamical descriptions of the system, and may be constrained by properties of individual SPPs. Further, there are useful generalities to arrive at through characterizing an active material's mesoscale structure in this way, or by classifying a material along this mesoscale dimension. There are population-density thresholds under which collective action fails to be directed, and over which there is not physical room or energetic availability for individual SPPs to produce sustained motion.

Second, in light of this first point, it is worth addressing a traditional means of characterizing active matter and active materials that I have, so far, consciously ignored. Frequently, the collective, directed activity of active materials is characterized as a form of emergence; indeed, this is discussed elsewhere in this special issue. While it is not a mistake to describe the macroscale behavior of active materials in this way, it is also not clear to me that this description is particularly productive for the purposes of characterizing or classifying active materials. Instead, I believe it is advantageous to construe the relations among parts exhibited in active materials as *inherently multiscale*, rather than simply emergent. Describing the relations among parts in active materials as “inherently multiscale,” rather than as “emergent,” suggests different ways of conceptualizing the interrelations among the parts, and behaviors of the parts, of an active material. That is, in investigating a particular behavior of a particular active material, asking, e.g., *whether* the behavior is an instance of emergence generates a different set of classificatory concerns than asking, e.g., *how* the behavior connects to behaviors at higher or lower scales.<sup>9</sup>

This philosophical reclassification reflects some of the present challenges of active materials research, which have mainly to do with reconciling the behavior of parts and their collections with behaviors of the whole material. As Batterman and Green (2020) argue, there is both scientific interest in and philosophical reason for attending to the behavior of mesoscale parts of active-matter systems in order to adequately capture patterns of generalities in complex systems. In active materials, over and above general issues of active matter, the mesoscale offers an additional locus for tuning and designing synthetic materials to suit the goals of a research project or application. Conceiving of mesoscale, SPP-population-level considerations as a dimension of active-materials classification will enable researchers to access design considerations more effectively,

<sup>9</sup> As an aside, here is an additional, somewhat speculative, rationale for this redescription: Philosophical discussions of emergence carry the baggage of the reduction/emergence debate, which, roughly, asks whether the properties or behaviors of wholes can or should be “reduced to” the behaviors of parts. Different parts of the debate spell out “reduced to” in different ways: some authors investigate whether the properties of wholes can be *explained* by the properties of parts; others inquire after whether the whole *exists* over and above the sum of the parts. In my view, this focus has led to overmuch emphasis on whether or not two levels of description can be connected in a particular (reductive) way, as opposed to how those connections work, more generally. I suspect that re-orienting such conversations away from emergence and toward the epistemology of multiscale modeling will provide more fruitful ways forward for moving away from “whether” and toward “how,” but a robust defense of this suspicion is a project for another day. I thank a reviewer for pushing me on this point.

and it will constrain the design considerations they give to both individual SPPs and material-wide dynamical descriptions. While there may yet be reason, philosophical or scientific, to continue analyzing the activity of active materials in the framework of emergence, it seems clear that for the sorts of classificatory purposes I am considering here, the conceptual tools of the multi-scale analysis outweigh those of emergence.

In the previous two sections, I developed reasons for conceptualizing active materials as synthetic kinds and explained what advantages accrue to developing specifically synthetic approaches to classification and characterization. In this section, I offered a further argument that the activity underlying active materials should be modeled as an instance of multi-scale material behavior, rather than emergent behavior. Due to these considerations, I believe it is productive and appropriate to conceive of active materials as inherently multiscale synthetic kinds. Before I conclude this discussion, I want to address one further classificatory distinction in the consideration of the classification and characterization of active materials, namely the role of (non-)equilibrium in defining, characterizing, and classifying active materials.

## 5 Smart materials, active materials, and equilibrium

The activity that defines active matter and active materials requires energy, which means that active-matter and active-material systems are necessarily out of thermodynamic equilibrium. Occasionally, this characteristic of active systems is explicitly referenced in descriptions of what makes an active system active, as in the following:

The ubiquitous nonequilibrium condensed systems that this review is concerned with have come to be known as active matter (Marchetti et al. 2013, p. 1144).

[M]icrotubules and actin filaments are fairly rigid linear structures, which are fundamentally out of equilibrium. Furthermore, they are structurally polar and provide a directionality for active processes (Prost et al. 2015, p. 111).

[In] the cellular cytoskeleton, cells and entire tissues are driven away from equilibrium by the continuous motion of thousands of constituent nanoscale molecular motors, protein-based machines that transform chemical energy into mechanical motion. Collectively, such microscopic activity leads to the emergence of new behaviours at each level of hierarchical self-organization, enabling the survival and reproduction of living organisms (Needleman and Dogic 2017, p. 2).

Each of these passages highlights the connection between the activity of active-matter and active-material systems and their status as non-equilibrium systems. The review articles, from which the first and third quotes are drawn, both explore this connection further, looking at the fundamentality of non-equilibrium processes in the very idea of a machine or a living system. Further, each of the articles quoted above reflects on the fact that active-matter and active-material systems are a special kind of non-equilibrium system, one in which the energy input that keeps the system out of equilibrium enters the system's dynamics at the level of SPPs. Marchetti et al. put the point thusly:



A distinctive, indeed, defining feature of active systems compared to more familiar nonequilibrium systems is the fact that the energy input that drives the system out of equilibrium is local, for example, at the level of each particle, rather than at the system's boundaries as in a shear flow. Each active particle consumes and dissipates energy going through a cycle that fuels internal changes, generally leading to motion. Active systems exhibit a wealth of intriguing nonequilibrium properties, including emergent structures with collective behavior qualitatively different from that of the individual constituents, bizarre fluctuation statistics, nonequilibrium order-disorder transitions, pattern formation on mesoscopic scales, unusual mechanical and rheological properties, and wave propagation and sustained oscillations even in the absence of inertia in the strict sense (Marchetti et al. 2013, pp. 1144–45).

Non-equilibrium status enters active matter and active materials at the microscale, through processes associated with SPPs. This makes active matter and active materials special kinds of non-equilibrium systems. On its own, this fact is not sufficient to offer any particularly interesting insights into the classification or characterization of active materials, save perhaps the general observation that it is possible to generate classification systems for SPPs according to types of the mechanics of energy consumption, and it is likewise possible to generate classes of non-equilibrium dynamical models that operate under the the constraint described in the passage above. These dimensions of classification may prove more for some purposes than structural or compositional approaches to classification, for instance in designing a material that metabolizes an energy source in an efficient or renewable manner. As scientists develop classification and characterization systems for active materials, being able to classify according to the particular ways that materials and their parts remain non-equilibrium will be an additional, potentially useful, tool.

In addition to these admittedly hypothetical considerations, there is a more immediate classificatory use of this insight about the particular ways in which active materials are non-equilibrium systems. The entry of energy into active materials through SPPs can be used to distinguish active materials from smart or responsive materials, which are a nearby class of synthetic kinds that face some similar design considerations to active materials. Smart materials, also known as responsive materials, are natural or engineered materials capable of exhibiting a designed response to stimuli that often involves the conversion of energy of one sort into another: piezoelectric materials produce electric voltage in response to mechanical stress; electroactive polymers change size or shape when electricity is applied; and smart inorganic polymers can release molecules in response to thermal stimuli, and self-repair.

A quite practical challenge of modern materials research is explaining the innovation in new engineered materials, and “smart,” “responsive,” and “active” are all contemporary buzzwords for materials design that can be applied to a range of industrial, medical, and other specialized engineered materials. These designations can become confusing for researchers, engineers, and consumers in border cases. I believe the foundations of classification developed here may help to resolve this challenge.

To make the challenge, and its solution, concrete, I consider the case of shape-memory alloys. The most common shape-memory alloys are nickel–titanium (NiTi-

NOL<sup>10</sup>) and copper–aluminum–nickel, but others exist. Shape-memory alloys are a class of alloys that can undergo plastic deformation below a certain temperature threshold and then be returned to an initial “remembered” shape upon heating. For instance, a shape-memory wire can be coiled into a spring, cooled, uncoiled, and returned to its coiled shape upon re-heating. This gives shape-memory alloys the ability to perform mechanical work. Further, that work is explained by appealing to the activity of microstructural features of the alloy, as the shape-memory effect is achieved through grain restructuring that occurs at particular temperature thresholds. In NiTiNOL, and some other shape-memory alloys, this restructuring is due to a transition between austenitic and martensitic metal phases, called hysteresis. The two phases orient atoms in a grain in differing relative positions with different symmetries and produce distinct associated macroscopic properties.

NiTiNOL and other shape memory alloys undergo dynamical activity due to the motion of microstructural material parts. Whether those parts count as SPPs depends on whether the question is being asked before or after a heat-induced or mechanically-induced hysteresis—in the immediate aftermath of a phase transition, before the alloy has achieved a steady-state in its new phase, there is a dynamically-relevant sense in which the individual atoms in a shape-memory alloy are acting as SPPs as they reorganize into their new grain structures. So, neither the description of the material as containing self-propelled parts, nor the description of it as undergoing macroscopic dynamical activity due to those parts, can discriminate in this case between an active material and the “smart” shape-memory material. However, the self-propelled parts in a shape-memory alloy are not consistently out of equilibrium; instead, their return to equilibrium in the new phase is what achieves the “activity” of the shape-memory effect. For this reason, being able to appeal to active materials’ special status as inherently non-equilibrium materials can assist in distinguishing active materials from smart and responsive materials. It may further be the case that appealing to the particular way in which energetic influxes enter active materials through SPPs can provide additional discriminatory capacities for other border cases.

Both smart materials and active materials are material classes of significant contemporary interest for their abilities to accomplish through material design work that was previously relegated to machines and fuel, and applications for smart and active materials range widely across energy storage, drug delivery, sensors, and more. As these technologies become increasingly prevalent in research, engineering, and application settings, having a principled means of classifying a material as either smart or active may assist in communication about both particular material designs and about the study of material behaviors. While this point does not fall strictly within the purview of the present discussion of classification and characterization of active materials themselves, it seems an advantage to be able to use the foundations developed here to venture outward onto the landscape of nearby materials classification concerns.

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<sup>10</sup> So named because the alloy was first synthesized by the U.S. Naval Ordnance Laboratory, NOL.

## 6 Conclusions

This discussion has aimed to provide some foundational themes for development in the consideration of how to classify and characterize active materials. One of my main aims was simply to distinguish active materials from active matter in a way that both captured existing distinctions in the way the terms are used and offered a rational basis for using one term over the other. In designating active materials as synthetic materials designed to exhibit active-matter principles, I hope to have achieved this aim. I would be remiss if I did not acknowledge a limitation of this proposal, which is that it does not adequately account for a common terminological move in both medicine and materials science, the designation of a material as “[x]-active”—surface-active, cathode-active, nano-active, etc. “Surface-active material” is a common enough phrase in medicine, where it is used interchangeably with “surfactant,” particularly in discussions of the composition of the lungs. Other “[x]-active” designations range across materials research, often in energy-storage contexts. This is an unfortunate double usage, especially as active materials hold some potential for energy-storage applications, but I do not consider it damning for the terminological proposal I make here.

With the terminological point established, the remainder of this article aimed at two main goals. First, I argued for a conception of active materials as synthetic kinds, which required some background discussion of what constitutes a synthetic kind and why it is productive to distinguish synthetic from natural kinds. Unlike most accounts of scientific classification, the account given here emphasized the partiality, context-sensitivity, and friendliness to cross-cutting classification available to synthetic classification systems.

Second, I used the advantages of the synthetic-kinds account to analyze three central dimensions of classification for active materials: (1) the structure and behavior of the self-propelled parts that comprise the microstructure of active materials, (2) the varieties of macroscopic dynamical activity produced by the aggregate behavior of self-propelled parts, and (3) the ways in which the self-propelled parts are driven out of equilibrium. During the course of my commentary on the first two dimensions, I also argued that it is at least sometimes advantageous to conceive of the activity of active materials as an example of multiscale material behavior rather than emergence. During the course of my commentary on the third, I also argued that the special non-equilibrium status of active materials should be used to distinguish active materials from smart and responsive materials in broader landscapes of materials classification. Throughout the proceedings, I have made use of a distinction between classification and characterization that I believe has not received sufficient philosophical attention as yet.

These remarks have been intended as initial formulations and foundations toward a system of classification for active materials. They have also been presented as a series of philosophical provocations, as I believe further reflection on a number of the topics covered here is still warranted. Some of that coverage is found elsewhere in this special issue, primarily on themes found in my discussion of multiscale material behavior. Other coverage, particularly of the nature of synthetic kinds and the classificatory considerations due to smart materials, will have to wait for another day.

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## Compliance with ethical standards

**Conflict of interest** The author declares that she has no conflict of interest.

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