Reconsidering Explanation: Lessons from Nanosynthesis

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Abstract

Nanosynthesis forces a reevaluation of received views on scientific explanation. I discuss the synthesis of anisotropic metal nanoparticles, a typical nanosynthesis research program, in order to demonstrate the failure of standard philosophical accounts of explanation to capture the dynamics of information exchange in synthetic sciences. I argue that using the language of *effective heuristics*, coupled with attention to changes in the meanings of concepts across different length scales, is a more promising means of capturing how information is obtained from the study of nanosynthesis systems.

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Explanation is a classic topic in philosophy of science, and for good reason. But little has been said about explanation when the aim of a scientific practice is production or synthesis—making something—rather than describing. Disciplines like chemistry, materials science, and nanosynthesis, which I will call the synthetic sciences, are interested in accomplishing different kinds of tasks than disciplines like theoretical physics and biology.

The aim of these disciplines is to make new substances and materials and to obtain scientific understanding through the process of production rather than observation or classification of pre-existing natural systems. And these disciplines aim to answer different kinds of questions to obtain scientific understanding; rather than answering questions about why something happens, the questions that the synthetic sciences aim to answer are more often questions about how to produce a new substance or material or why changing a procedure results in an altered product.

Most theories of explanation, whether they are deductive-nomological, unificationist, causal-mechanical, or pragmatic, have not addressed the role of explanation in the synthetic sciences. And it seems remiss that philosophers have failed to account for explanation in chemistry, one of the big-three natural sciences, which is supported by some of the largest scientific societies in the world. Articles made up of descriptions of synthetic procedures, and discussions of how these procedures produce new substances and materials with new and interesting properties, occupy the bulk of most chemical

journals. These articles add to the collective base of scientific knowledge, the information one might turn to in order to answer questions about why and how the world works in the ways that it does. So in this minimal sense, at least, the information that moves the synthetic sciences forward is explanatory. It is thus worth considering how this information works, in order to sketch a view of what a theory of explanation in synthetic sciences might look like.

This talk considers explanation in nanosynthesis, a branch of chemistry that aims at making nanoscale materials. I borrow the language of a variety of theories of explanation in order to accomplish this task. I have already framed the problem in terms familiar to van Fraassen's why-questions account. Hacking's and Woodward's interventionism will appear later, as will some of the explanatory strategies that Batterman describes in The Devil in the Details and later work. Influences from confirmation theory and from Wimsatt's theory of heuristics also influence my attempt to sketch a philosophical account that captures the structure and function of explanation in nanosynthesis. Sometimes these other accounts succeed at capturing an aspect of explanation in nanosynthesis; elsewhere they fail or, more commonly, they simply fall silent.

I begin by introducing the notion of an *effective heuristic* to describe how explanation works in synthetic sciences. Effective heuristics are well-confirmed strategies for reliably reproducing a particular kind of behavior in the interaction of two or more substances or materials. In chemistry, effective heuristics tend to be rules about the reactivity of substances.

I borrow the language of heuristic from William Wimsatt, whose extensive characterization of heuristics appears in an essay entitled Heuristics and the Study of Human Behavior. While Wimsatt uses the term as a contrast to **algorithm**, which does not concern me here, his aim in introducing the term is to provide an alternative to reductive accounts of explanation in science.

One of the upshots of my account is that effective heuristics are distinct from, and neither superior nor subservient to, traditional explanatory strategies that make heavier use of theoretical justification. In this way the account of explanation I advocate is a kind of pragmatic pluralism. Sometimes causal stories will most effectively explain a situation; other times unifying stories will. In synthetic situations, however, heuristic stories often, if not always, provide the best explanation of how to carry out a procedure. I hope to show that even if one were equipped with a robust theory of the mechanics and reactivity in nanoscale systems, one would still need explanations in terms of effective heuristics to guide synthetic practice.

As an example of an effective heuristic in chemistry, take the rule that alkali metals tend to combust in water, and that heavier alkali metals such as potassium combust more violently than lighter metals like lithium. This rule is distinct from, but related to, the theory that would explain the combustion in terms of the dynamics of electrons and chemical bonds. Note that effective heuristics are effective because they are particular to a certain class of substances, and generalization of these heuristics frequently leads to a decrease in their effectiveness. For instance, there is no effective heuristic about

the behavior of *all* metals in the presence of water.

Generalization and mark-transmitting causation are not the goals of heuristics; rather, the rules are developed in order to guide future syntheses, and as a kind of justification of syntheses that have been performed. They may be indicative of natural phenomena that are explainable in D-N, unification or mark-transmitting causal terms, but they themselves are not necessarily D-N, unifying, nor mark-transmitting, although they might fit under a broad reading of Woodwardian-style interventions.

For the remainder of this talk, I aim to illustrate how effective heuristics work. More than one heuristic is required to perform most syntheses of interest, and the relationships between multiple heuristics, as well as between heuristics and theory, have not yet been made clear.

I am interested in the interaction of the heuristics involved in an explanation of a nanosynthesis procedure, because understanding this interaction will help both philosophers and scientists to see how explanatory information is developed across a variety of theoretical models and over a variety of scales.

In order to clarify this point, it is necessary to review some of the heuristics involved in a common nanosynthesis procedure, namely the synthesis of anisotropic metal nanoparticles, or AMNPs. AMNPs are single-crystalline particles with recognizable, non-spherical geometries such as cubes, octahedra, triangular plates, or elongated wires. They are of particular interest for their potential applications in fields as diverse as drug delivery, cancer therapy, optics and electronics. Gold nanocubes like the ones on the slide, for instance, can be activated by infrared lasers to cause highly localized cell death in a micrometer radius, and thus kill tumors without exposing the whole body to either poisonous chemicals or harmful radiation.

There are multiple methods available to synthesize AMNPs, and here I will only review one of the most common, which is known as synthesis via wet chemistry. It begins by combining two liquid solutions in a standard reduction-oxidation or acid-base reaction, which results in elemental metal precipitating out of solution. Then nanoparticles begin to nucleate and grow. Next a capping agent is added, a substance that constrains the size and shape of the nanoparticles as they continue to grow. These steps can occur either in one single reaction or in two or more reactions. Finally, the procedure is repeated with variations in order to *tune* the size and shape of the particles to obtain the desired response.

In either case, the heuristics that guide decisions about how to proceed at the first stage of the synthesis are grounded in reduction-oxidation theory and/or acid-base theory, which are orthodox chemical reaction theories that were developed to explain reactions in bulk matter. These theories predict, and experiment confirms, that elemental metal will precipitate out of solution by the reduction of cationic metals, via an added solution of a reducing agent. So for instance a heuristic at this stage is that increasing the concentration of the reducing agent will make the reaction proceed faster. This rule is grounded in chemical reaction theory, which explains why metals reduce faster in the presence of more molecules of a reducing agent. But the rule itself explains how to get an actual sample of metal into an environment where there are

more reducing-agent molecules around.

Once precipitated, elemental metal self-assembles in the reaction solution to form spherical seed particles. This process is called nucleation. The size of nucleated seeds can vary greatly within a given reaction, as well as from one reaction to the next. Heuristics that guide the control of seed size are also rules about changing the concentration or time of a reaction, but they are justified by a very different theory, one that makes radically different assumptions about the nature of the materials in the reaction.

This theory is known as LaMer theory, after its founder. It treats small bodies in solution as continuous, smooth and perfectly spherical objects that grow at different rates based upon the amount of time the reaction spends in a high-concentration state known as supersaturation, which is indicated by the topmost region in the graph on the slide. The longer a reaction spends in supersaturation, the less uniform the final distribution of nanoparticles will be, because new particles will continue to nucleate while older particles grow. Further rationales for this phenomena in terms of the energetics of nucleation are also part of LaMer theory. In terms of the effective heuristic for this stage of synthesis, manipulating the concentration of various substances in a given reaction will affect the amount of time the reaction spends in supersaturation.

Unlike redox theory, LaMer theory does not work for macroscopically-sized bodies, and it does not refer to the atomic nature of the materials involved or to chemical reactivity. So moving from the first heuristic at the first stage of AMNP synthesis to this second heuristic actually indicates a large shift in theoretical context; that is, a shift in the information needed to move forward with the synthesis. It seems natural to consider shifts of this sort as changes in explanatory context as well.

For reasons that will become clear shortly, I call moves of this sort *scale-dependent assumption shifts*. Scale-dependent assumption shifts are the answer to the question of how heuristics interact with each other and with theory in nanosynthesis in order to provide robust explanations of synthesis procedures.

Scale-dependent assumption shifts are defined by changes in the relevant behaviors of interest in the system, accompanied by changes in the assumptions required to theoretically model the system. These moves are scale-dependent in the case of nanosynthesis because the behaviors of interest occur at different length scales during each stage of the synthesis procedure. Shifting attention from what is happening at a macroscopic scale to what is happening at the nanoscale is what allows chemists to collect and apply the information needed to perform the synthesis, and to obtain and use effective heuristics that can guide future procedures.

Moving to the third stage of AMNP synthesis will round out the example and demonstrate two further cases of scale-dependent assumption shifts. It is necessary here to understand that nanomaterials are highly unstable compared to macroscopic materials, because more of their atoms are on the surface of the material and consequently bonded to fewer other atoms in the material. So nanomaterials require stabilization.

In the third stage of AMNP synthesis we are considering here, a capping agent is introduced to the reaction pot in order to stabilize the particles. A useful analogy is

to think of capping agents as a kind of sausage casing that holds the atoms of the nanoparticle in place. Capping agents prevent nanoparticles from growing above the nanoscale, as they would tend to do otherwise, and some capping agents also control the shape of the final particles by attaching selectively to one crystal facet or another. So heuristics that guide this stage of AMNP synthesis identify particular capping agents as better or worse for producing a desired shape in a given substance.

The reason this move counts as a scale-dependent assumption shift is because of a change in the theoretical context needed to understand why different capping agents produce different shapes. This stage of the synthesis actually witnesses two such shifts within various parts of crystallographic theory.

The theory of Miller indices associates different crystal facets with different vectors, and assigns different energies and chemical affinities to different crystal shapes based on the results of this vector analysis. Here crystals are treated first as ideal geometric bodies. Then, in order to accommodate the action of the capping agent itself, crystal surfaces are re-conceived as entities made up of atoms packed together in different arrangements with different available sites to bond with the capping agent.

Now that I have shown how effective heuristics and scale-dependent assumption shifts work in the context of explaining AMNP synthesis, I will draw out some conclusions about the structure and function of explanation in nanosynthesis. To review, each stage of AMNP synthesis is accompanied by an effective heuristic that indicates how to proceed to obtain the desired result at that stage. As a reminder, the slide illustrates each stage of synthesis and the heuristic at play during that stage. At the beginning of this talk I argued that this kind of information counts as explanatory because of its role within the synthetic-science community. This kind of information both contributes to chemists' understanding of the systems they study as well as guiding further chemical practice.

Moreover, the kind of information carried in effective heuristics defines the very practice of chemistry, and all synthetic sciences. So even if purists about explanation reject effective heuristics as a form of explanation, these heuristics are *still* a central part of a widespread and successful theoretical practice that philosophers of science have, so far, failed to account for.

While few if any philosophers have written specifically on explanation in the synthetic sciences, quite a few have written on the role of scales in explaining various physical and biological phenomena. While time does not permit me to give a full overview of all the existing views, I would like to review the three that I find most promising and most relevant to the treatment of scales I have given here.

Firstly, in 2006 Mark Wilson labeled the move from one theoretical context to another *physics avoidance*, and he has more recently written about scale-dependence in classical mechanical systems. But the term physics avoidance does not capture either the scale-driven motivations for shifting assumptions or the widespread existence of this shift in domains besides physics. Scale-dependent assumption shift is nowhere near as catchy a term, but it captures the essential notion of changes in theoretical contexts resulting from changes in the scale at which a system is studied and implying changes

in the relevant concepts, data, and behaviors being considered in the study of the system.

Also in 2006, Eric Winsberg elaborated on modeling strategies that rely on scale-dependent assumption shifts, although he did not call them as such. His *handshaking* models interact in dynamic feedback loops to produce holistic descriptions of systems that could not be built from one theoretical model alone, nor from a series of models applied in sequence. While Winsberg captures both the scale-dependence and the interactive interplay of theoretical contexts needed to explain nanoscale systems, his account has not explicitly addressed the particular challenges of explaining synthetic systems at the nanoscale.

Earlier this year, Bob Batterman discussed the role of scales in explanation in the physical sciences at length in an article entitled The Tyranny of Scales. His interest, continued from his 2001 book, is in how explanations of physical phenomena are built in situations where multiple scales are required to model the system. His work focuses primarily on mathematical models of physical systems and engages with materials-science literature on multi-scale modeling. In particular, Batterman's interest in describing how explanations of phenomena like the bending of steel can, quote-unquote, bridge across scales closely relates to my own interest in describing how explanations of syntheses arise from the interactive interplay of effective heuristics at different scales.

So, I am not the first to point out that scales play an important role in philosophical accounts of explanatory strategies. But nanoscience provides a particularly striking example of scientific systems that are not only sensitive to scale but also defined by scale. And nanosynthesis introduces the additional explanatory demands imposed by synthetic sciences, those parts of scientific practice whose aims are production, over and above description.

This talk represents a first attempt to construct a philosophical account of explanation in synthetic sciences, using the example of nanosynthesis. My strategy has been to pay close attention to what kinds of information nanochemists need in order to understand their systems better and to make nanoparticles more effectively. Perhaps unsurprisingly, explaining nanoscale systems requires awareness of, and movement between, theoretical models that describe matter at a variety of scales. But explaining the synthetic aspects of these systems also requires information about how synthesis procedures are carried out. And I have argued that effective heuristics play an integral and, up to now, unrecognized, role in explanations in the synthetic sciences. It is time for that to change.

Thank you.