Surface Tension: Conceptual Challenges in Modeling Nanoscale Material Surfaces

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Abstract

All solid and liquid materials have surfaces, and surfaces typically exhibit different physical and chemical properties and behaviors than the bulk or interior of the materials they contain. The properties and behaviors of surfaces are, thus, a universal feature of materials and a perennial object of study in the physical sciences. One important way in which this study manifests is in the modeling of materials. Contemporary philosophy of science has taken a strong interest in the epistemology of scientific modeling, and recently, particular attention has been given to the conceptual, epistemic, ontological, and practical challenges posed by multiscale modeling. Representing surface properties and behaviors within a wider context of material behavior is often a goal of constructing multiscale models of materials. Despite this, and despite that much philosophical literature on multiscale modeling addresses models in physics, little has so far been said about the challenges associated with modeling material surfaces. Further, nanoscale materials present a variety of practical, theoretical, and conceptual challenges for traditional approaches to modeling the physical and chemical behavior of materials. In this article, I examine how two distinct approaches to modeling surfaces arise from two distinct conceptions of what a surface is. I call these the "boundary on a body" conception and the "outermost layer" conception, and I show how the distinction both underwrites different modeling strategies and threatens reductive approaches to the epistemology of modeling.

1 Introduction

All solid and liquid materials have surfaces, and surfaces typically exhibit different physical and chemical properties and behaviors than the bulk or interior of the materials they contain. The properties and behaviors of surfaces are, thus, a universal feature of materials and a perennial object of study in the physical sciences. One important way in which this study manifests is in the modeling of materials. Models of surface properties and behaviors differ from models of bulk properties and behaviors of the same material; additionally, modelers face practical, epistemic, and ontological challenges in how to represent surfaces within models of bulk materials. Many of these challenges arise from an apparent contradiction in the way that surfaces are modeled: surfaces are variously modeled as both reduced-dimension boundaries on the bodies they contain, and as extended material components of bodies, with internal structure and dynamics of their own.

Contemporary philosophy of science has taken a strong interest in the epistemology of scientific modeling, and recently, particular attention has been given to the conceptual, epistemic, ontological, and practical challenges posed by multiscale modeling. Representing surface properties and behaviors within a wider context of material behavior is often a goal of constructing multiscale models of materials. Despite this, and despite that much philosophical literature on multiscale modeling addresses models in physics, little has so far been said about the challenges associated with modeling material surfaces. Further, nanoscale materials present a variety of practical, theoretical, and conceptual challenges for traditional approaches to modeling the physical and chemical behavior of materials. One significant source of these challenges arises from the influence of surface behavior on the material behavior of nanomaterials. Nanoscale surfaces are non-negligible parts of the materials to which they belong. As such, modeling, controlling, and understanding the behavior of surfaces is crucially important to modeling, controlling, and understanding the behavior of nanomaterials as a whole.

In this article, I examine how two distinct approaches to modeling surfaces arise from two distinct conceptions of what a surface is. I call these the “boundary on a body” conception and the “outermost layer” conception. In Section 2, I explicate the distinction between the two conceptions of a surface. The next two sections offer case studies showing that these two conceptions can come into tension in materials modeling scenarios. Section 3 illustrates how these two conceptions are both used in the modeling of fluid flow with boundary-layer theory. Section 4 introduces the reader to the special problem of conceptualizing and modeling nanoscale surfaces, which I argue threatens the “boundary on a body” conception of surfaces. Section 5 provides a more in-depth analysis of the two conceptions and argues that each conception is associated with distinct modeling strategies, which are loosely affiliated with distinct disciplinary approaches to modeling. In section 6 I discuss a final case study of a nanomechanics experiment, in which a stalled experimental protocol was restarted by shifting from one surface modeling strategy to another. Section 7 offers final remarks on the prospects for resolving the apparent tension between the two conceptions of surface. These include an argument against a reductive resolution to the problem and a critique of Mark Wilson’s account of “conceptual multi-valuedness” [42] as a contextual alternative to reductive approaches. I conclude that the two conceptions of a surface stand in a scale-dependent relationship to one another, and that changes in scale can and should motivate changes in modeling strategies.

Before I proceed further, it should be noted that the subject of this discussion is models of material surfaces. By “material surface” I here mean the outermost portion of matter in bodies or materials. No solid or fluid object exists without being bounded by a material surface. Material surfaces are often detectable by plain touch or sight, or by measuring

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changes in dielectric constant, refractive index, crystal lattice, or other physical properties that result at the interface between two physical or chemical phases. Material surfaces are comprised of collections of atoms, and as such they are distinct from the electron-shell surfaces depicted as attaching to a single atom in space-filling diagrams of atoms and molecules. They are, likewise, distinct from, but related to, dielectric interfaces more generally. The relation between material surfaces and electronic surfaces is non-trivial and beyond the scope of the present discussion. For the sake of relative brevity, I use “surface” interchangeably with “material surface” here, unless otherwise noted.

2 On Two Notions of a Surface

Centuries ago, in developing his physics and metaphysics, Descartes encountered difficulty in defining the notion of a surface to the satisfaction of his contemporaries. In the sixth set of objections to his *Meditations*, Descartes’ interlocutors ascribe to him the view that surfaces are the place where sensation occurs, and they inquire how he distinguishes the surface from both the body and the environment of an object. Descartes replies:

> I conceive of the surface by which I think our senses are affected no differently than all mathematicians and philosophers normally conceive of it. They distinguish it from the body and suppose that it lacks any depth. However, the word “surface” is taken in two senses by mathematicians. In one sense, they use it to refer to a body to whose length and breadth alone they direct their attention and which is viewed without reference to its having any depth, although they are not denying that it does have some or other depth. In the second sense, they use it merely to refer to a mode of a body, that is, when all its depth is denied. [14, p. 199–200]

In this reply, Descartes aims to disambiguate between two ways of understanding surfaces. In the first, surfaces are bodies that derive their mathematical and physical interest from length and breadth alone; that is, they are bodies whose depth is uninteresting or unimportant for any mathematical or physical modeling, or philosophical speculating. In the second conception, surfaces occupy a distinct ontological category from bodies; they are modes, or boundaries, on bodies, depth-less outer limits that differ in kind from the sort of objects they contain. Descartes goes on to affiliate his own writings with the second conception.

This distinction is perhaps not original to Descartes, and on its own it does not constitute a significant tenet of his physics or metaphysics. Nonetheless, contemporary materials modeling continues to employ both conceptions of surfaces, often without acknowledgement of the distinction and sometimes in the modeling of a single material. This generates an apparent contradiction in the way surfaces are represented in contemporary models of materials.

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I will call the two conceptions of surfaces the "outermost layer" (hereafter OL) conception and the "boundary on a body" (hereafter BB) conception, respectively. These two conceptions, or notions, of a surface generate distinct modeling strategies, which I discuss in more depth in Section 5. An essential difference between the two conceptions is that the OL conception generates models of surfaces in which surfaces possess depth, which gives rise to the possibility of internal structure and dynamics within a surface. The BB conception, on the other hand, treats surfaces as reduced-dimension boundaries with no internal structure. By far, the most common two strategies for modeling material surfaces consist either in (i) developing a structural model of the parts and behaviors of a material surface, or in (ii) either parameterizing or ignoring the effects of a surface in order to model the overall behavior of a material.

The former strategy is successful in contexts where micro-scale chemical or physical behavior is a primary target of the model, whereas the latter is successful in contexts where the surface is modeled as a constraint on larger-scale material behavior. In this way, the OL conception of surface is favored in micro-scale modeling of surfaces, while the BB conception is favored in macro-scale modeling. For modeling of macroscopic materials, the two conceptions of a surface can generally be neatly separated out into distinct modeling contexts due to the large scale separation between the interior bulk of the material and its surface. The success of scale-separation strategies in physical modeling has been the subject of a number of recent philosophical accounts of multiscale modeling in natural sciences (e.g. [1, 43, 19, 37]), and some (e.g. [16, 6]) have even suggested that scale separation provides a new resolution to traditional worries about reduction and emergence.

In Section 3, I illustrate how scale separation can resolve the apparent tension in the two conceptions of surface in the case of modeling boundary layer flow in fluid mechanics. Then in Section 4, I explain how the need to model nanoscale surfaces poses a challenge for resolving the apparent tension between the two notions of a surface through scale-separation alone.

3 Boundary Layer Flow Modeling: Two Conceptions, One Problem

As a canonical example of the sort of modeling scenario where both the OL and BB conceptions of surfaces arise, consider the modeling of boundary layer flow in fluid mechanics. The modeling of boundary layer flow has already found its way into the philosophy of science literature, particularly in the work of Margaret Morrison [29, 30, 32] and Mieke Boon [4, 5]. In boundary layer flow modeling, a need arises to model a surface as something that is both a boundary on a body, and as something that has depth and texture of its own. The philosophical puzzles raised by boundary layer modeling run the gamut from worries about model ontologies and the nature of representation to the relation between model and experiment, and between physical models and mathematical models. These are

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discussed at length in responses to Morrison's view (e.g. [4, 17, 30, 40, 32]), as well as in [12, 3, 1, 34].

In the latter parts of the 19th century, physicists faced a problem in modeling fluid flows, namely that the best mathematical model of fluid motion, the Navier-Stokes equations, were unable to provide exact solutions for viscous fluids.[1] In the early 20th century, Ludwig Prandtl proposed a solution in the form of his boundary-layer flow equations. This mathematical model "compressed" information about the motion due to fluid friction — that is, viscosity — into the mathematical representation of the layer of fluid immediately adjacent to the solid boundary through which the fluid flowed. This meant that the remaining interior bulk of the fluid could be modeled with Navier-Stokes dynamics. Prandtl's boundary-layer theory thus simplified the difficult problem of obtaining solutions to the available mathematical models of fluid flows.

In her account, Morrison describes Prandtl's work as "develop[ing] a kind of conceptual model of the fluid as consisting of two parts, the thin layer in the area where friction plays an essential role (the boundary layer) and the region outside where these effects can be neglected." [30, p. 82] I follow Morrison here in explicating the component models in the Prandtl model as ones that neglect vs. attend to friction, by which she and I both mean the effects of viscosity in the boundary layer flow. In the Prandtl model, the boundary flow has its own native dynamics, distinct from the bulk flow. In particular, the fluid behavior in the boundary layer is significantly impacted by the no-slip condition, which requires a zero flow velocity at the solid edge of the boundary layer.

In an influential discussion of the no-slip condition, Michael Day [13] reviews a variety of justifications for the no-slip condition. In this review he highlights the appeal to intermolecular forces as characteristic of most justifications of no-slip. The intuitive idea is that there are electrostatic forces between the solid boundary and the first fluid atoms in contact with it (adhesion forces), which overwhelm the weaker intermolecular forces (cohesive forces, e.g. van der Waals forces) and cause "sticking" of the fluid at the boundary. In a footnote, he points to a particularly evocative example of this type of reasoning from an article on numerical simulation model of boundary layer flow: "the no-slip boundary condition is a natural outcome of the interaction between the molecules of a solid and the fluid." [20, p.19]

This justification for the no-slip condition draws on the OL conception of surfaces, in particular of the surface of the fluid. To understand no-slip as a product of force-wise interactions between atoms in different materials is to give internal structure to the parts of the surface layer, such that individual interactions among atomic components are possible. As with the Langmuir and TSK models, the concept of atomic interaction via electron exchange is retained from the bulk to the surface, and that retention then licenses the use of the no-slip condition. However, the mathematical models most closely associated

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[1] This presentation draws primarily from [29] and [12], and has benefitted from conversations with [blinded for review].

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with boundary layer modeling (the boundary-layer flow equations) are a simplification of the Navier-Stokes equations. The simplification is achieved via an order-of-magnitude analysis, which requires the assumption that the length scale in which the boundary layer dynamics occur is significantly larger parallel to the direction of flow than perpendicular to the direction of flow. The order-of-magnitude assumption derives from the BB conception of a surface, which emphasizes the reduced dimensionality of surfaces relative to the bodies they enclose.

To sum up the problem, the no-slip condition was justified by the OL conception of surfaces, but the derivation of boundary-layer equations was justified by the BB conception. The two conceptions of surface contradict one another in their understanding of the existence of depth and, thus, internal structure, in surfaces. They have generated two modeling strategies, both of which are employed successfully to generate models of boundary layer flow. So, out of two apparently contradictory conceptions, both alike in fundamentality (in fair fluid mechanics, where we lay our scene), a pair of modeling strategies take their life. And unlike certain star-crossed lovers, the no-slip condition and the boundary layer equations survive and thrive together in boundary layer modeling. How can this be? Whither the contradiction, and why should we trust the resulting models?

As I gestured at above, the answer lies in recognizing that the two conceptions operate on different length scales of the system. In this case, the scale at which the BB conception operates is orders of magnitude larger than the scale at which the OL conception operates. The boundary layer equations are derived by “zooming out” and comparing scales between the whole bulk of the system and the boundary layer area, while the no-slip condition is justified by “zooming in” to consider individual interatomic interactions. Separating the scales at which these conceptions operate in this case then suggests that it may be fruitful to think of the resulting boundary layer model as a multiscale model, which allows us to address the problem above using readily available tools for unpacking the epistemology of multiscale models, such as [44, 1, 16, 43, 6, 32, 19].

4 The Novelty of Nanoscale Surfaces

Nanoscale materials are generally understood to be engineered or naturally-occurring materials with at least one dimension in the nanoscale, that is, between 1–100 nm. A nanometer is 10^{-9} meters, or one order of magnitude larger than the ångstrom, which is the SI unit used to measure distances in interatomic bonds. Researchers are interested in nanomaterials because nanomaterials exhibit different properties than macroscopic materials made of the same matter, such as increased catalytic activity, unusual combinations of strength and density, and various electromagnetic and luminescent phenomena.

Nanoscale surfaces differ from the surfaces of macroscopic materials in three important ways: they occupy a significantly greater proportion of the material, they exhibit properties that cannot be reproduced in the surfaces of macroscopic materials, and they require

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physical or chemical stabilization. For present purposes, I focus only on the first difference. Even in very small macroscopic materials, the quantity of atoms that comprise the interior of a material vastly outnumbers the quantity of atoms that comprise the material surface. Figure 1 illustrates the dramatic shift in proportion that occurs at the nanoscale. In the figure, the diameter of an approximately spherical cluster of palladium atoms is plotted against the percentage of atoms on the surface of that cluster. The reference point on the far right is for a bulk cluster with a 63 μm diameter — a spherical cluster with a diameter around the same size as the average diameter of a human hair. At this scale, the authors estimate that a negligible proportion of atoms[2] of the atoms in the cluster are on the cluster's surface. However, in the three marked points within the nanoscale, a substantial proportion of the atoms, even in a solid spherical cluster, are on the surface. From right to left, a 3.37 nm-diameter cluster is made up of about 35% surface atoms; a 2.5 nm-diameter cluster is made up of about 45% surface atoms; and a 1.2 nm-diameter cluster is made up of about 76% surface atoms.

Some nanomaterials, such as graphene or thin-film composite membranes, are made up almost exclusively of surfaces. In these materials, nearly every atom in the material lies in an interfacial region, that is, at the outermost layer of the material. The same might be said for single-walled carbon nanotubes, which are hollow straws of hexagonally-packed carbon. In these materials there is even an "inside" and an "outside," so there are two distinct interfacial regions (inside the straw and outside the straw) that display properties distinct from one another, as well as being distinct from the properties of the tube itself. Even for nanomaterials that are not comprised entirely of surfaces, the surface layer of atoms no longer occupies a negligible proportion of the material.

The difference in the relationship between a bulk material and its surface, and a nanomaterial and its surface, is like the difference between coating a baseball in grains of sand and coating it in ping pong balls. The latter poses challenges that are simply irrelevant to the former, such as how to measure the diameter of the ping-pong coated baseball (From the center of the ping-pong balls? From the outer edge? Somewhere in between?), how to pack the ping pong balls around the baseball most efficiently, and how the entire ping-pong ball coating will be affected if one more ball is added or taken away from the set. Questions analogous to these, concerning the measurement of surface properties of nanomaterials, comprise significant domains of nanomaterials research (For instance, see [15, 27, 18, 10, 26]).

Treating surfaces as boundaries on bodies, particularly by modeling surfaces as mathematical boundary conditions, has been a remarkably successful strategy in the modeling of bulk materials. The success of this strategy has been a subject of philosophical investigation and a source of insight into the epistemology of modeling (e.g. in [29, 4, 35, 1, 31, 43, 7]).

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[2] The authors describe the proportion as, " 0%" [33, p. 246]. A back-of-the-envelope calculation taking into account the protein structure of human hair, suggests that the proportion of surface atoms in a cross-section of a 50-μm strand of human hair can be estimated at roughly one in every 110,000, or around 0.0009%.

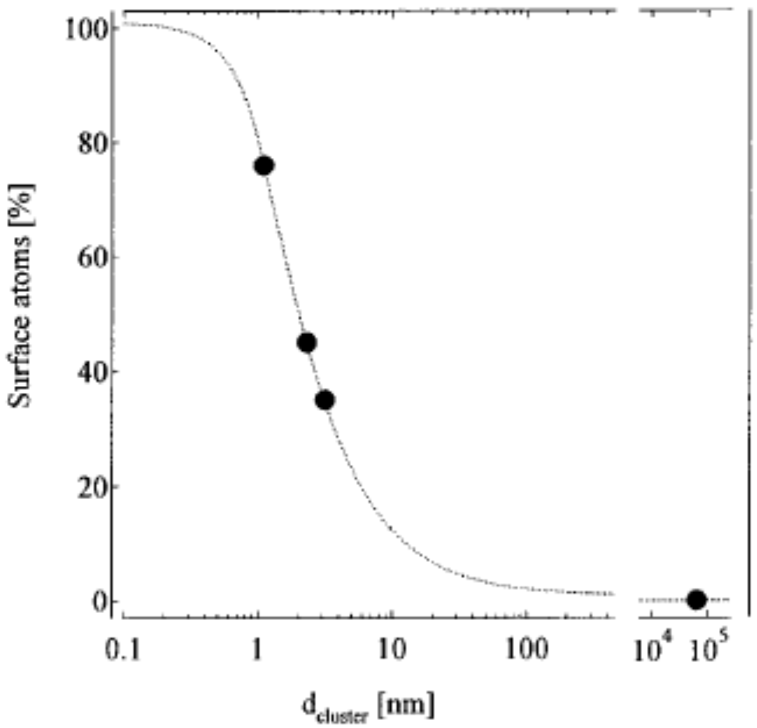

Figure 1: Diameter of an approximately spherical palladium cluster plotted against the percentage of atoms on the surface of that cluster, from [33]. From left to right, marked points lie at 1.2 nm diameter, with 76% surface; 2.5 nm diameter, with 45% surface; 3.37 nm diameter, with 35% surface; and 63 μm diameter, with negligible surface.

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That this strategy generates a conceptual conflict with the strategy of modeling surfaces as the outermost layer of materials has, conversely, gone largely unnoticed in such discussions. In the following Section, I elaborate upon the conceptual distinction between the OL and BB conceptions of surfaces and explicate the distinct modeling strategies that each conception generates. Then in Section 6, I use this distinction to articulate conceptual strategies for modeling nanoscale surfaces, and I discuss a case in which failure to adhere to these strategies had not only conceptual, but also practical consequences in the design of nanomaterials experiments.

5 Two Strategies for Modeling Surfaces

Here I argue that the OL and BB conceptions of surface each generate their own distinctive modeling strategies, which I call structural and parametric modeling, respectively. Structural models are loosely affiliated with chemical interests in modeling, and parametric with physical, but these are not hard and fast associations. The contrast between the structural and parametric approaches to modeling surfaces is best shown by a short series of examples. I have selected structural models that are central to contemporary surface modeling of nanomaterials, namely the Langmuir isotherm and the Terrace–Step–Kink model, and parametric models that are familiar in the philosophy of physics literature, namely acoustic modeling of vibrating strings. I show how the respective conceptions of surface associated with each model case are essential to the development of the models.

5.1 Structural Models of Surfaces

The Langmuir adsorption model [23, 24] is an example of a type of surface model that I will call "structural models of surfaces," due to this model type's emphasis on the parts and dynamics within a material surface. The Langmuir model aims to generate a mechanism for adsorption. Adsorption is the increase in concentration of a substance at a phase boundary due to surface forces. The Langmuir model supposes a flat (planar) surface with discretized adsorption sites, distributed evenly throughout the surface. In effect, it lays a lattice over a surface. Each adsorption site may be either occupied by a single adsorbate, or unoccupied. The dynamics of the model relate the partial pressure of the free (un-adsorbed) gas to the volume of gas that has been adsorbed and the proportion and volume of occupied adsorption sites. The model is used to study the interaction between the adsorption layer and the gas phase in its environment. The adsorption lattice is not intended as representative of the distribution of actual atoms in a material surface, although relations between an adsorption lattice and a crystal lattice may be studied.

Another structural model of surfaces is the Terrace–Step–Kink (TSK) model (also known as the Terrace–Ledge–Kink model), depicted in Figure 2 and originated in [21, 41] as an extension of Bravais-lattice models of crystal structure. The TSK model is a discrete model of surface structure and behavior, initially developed for modeling crystal surface

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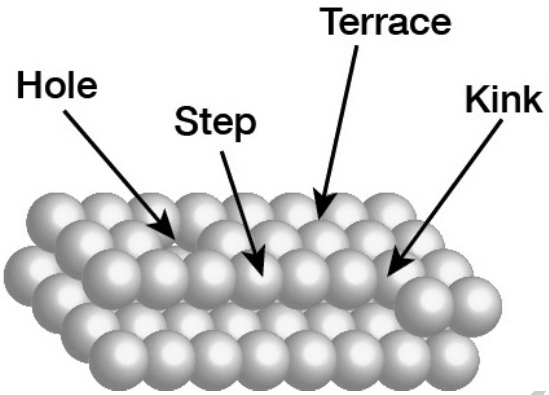

Figure 2: Schematic of four site types on a surface in the Terrace–Step–Kink model. Flat surfaces contain terrace sites. Edges where planes cleave make up step sites, and corners make up kink sites. Hole sites are individual removals of an atom in a plane. This figure is the author's rendering; the diagram structure is stereotypical to textbook presentations of TSK.

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structures. It assigns to different sites on a surface different thermodynamic properties, based on the presence or absence of atoms in the immediate environment of the site. Terrace sites are planar, with a site fully surrounded by in-plane neighbors. Step sites have in-plane neighbors on on side only. As a result, they are bound to the material they enclose by fewer neighboring bonding sites; atoms in step sites are less strongly attached to the material than atoms in terrace sites, which are less strongly attached than interior atoms. This makes atoms located at step sites higher-energy, which increases the reactivity, and thus decreases the stability, of the surface at that site. Other site types, such as corners and edges, are even higher-energy and even less stable than step sites.

Both the Langmuir adsorption model and the TSK model discretize surfaces in order to study chemical interactions on the surface of a material. Both are chemical models of surfaces developed to assist in the study of the dynamics of particles chemically interacting with surfaces. The Langmuir model was developed by Irving Langmuir in the late 1910s[24] and is often cited as part of the work on surface chemistry that earned Langmuir the 1932 Nobel Prize in Chemistry. The TSK model is usually attributed to work developed by Walther Kossel in the 1920s[21]. Kossel was a physicist by training, but he is best known for innovation in chemical bonding theory, as he advanced a version of the octet rule of ionic bonding with the same principles and in the same year as G.N. Lewis. Both in terms of history and in terms of scientific content, these two structural models are chemical.

There are many variations and extensions of adsorption models like the Langmuir model, and analogous variations and extensions of the TSK model into models of inhomogenous surfaces. Extensions and analogues of the Langmuir and TSK models appear across industrial, agricultural, organic, and inorganic chemistry. What models of this sort share in common is a localization of surface phenomena to particular sites on a material surface. This localization of possible sites of activity is a logical precondition for the study of localized behavior on surfaces, including adsorption, catalysis, and molecule and crystal growth. These surface phenomena comprise much of surface chemistry, and both adsorption and TSK models are both historically and presently predominant in chemical, as opposed to physical, models of surfaces.

That structural models of surfaces pervade chemistry should come as no surprise, since surfaces are where chemical reactions happen in materials. Much like it is impossible to reach a friend in the middle of a crowded room without first pushing past the people on the edges of the room, it is impossible for a chemical reaction to take place on the interior of a material without first taking place on its surface. Interior atoms are physically screened off or blocked from interaction with new chemical species by the presence of nearby atoms. Additionally, the fact that surface atoms are not bonded to or coordinated with as many atoms as an interior atom means that they have greater availability in their electronic structure to support the formation of new chemical bonds.

5.2 The Outermost-Layer Conception of Surfaces

Structural models are chemical. They are also, I contend, borne of the outermost-layer conception of surfaces. The OL conception posits that a surface on a three-dimensional material possess extension in the third dimension, or depth; or, at least, that it is not strictly necessary that surfaces do not posses depth. In the Cartesian supposition, and in much of contemporary science, this depth is not often considered to be a central or interesting aspect of the surface being modeled; it is frequently not mathematically represented as a variable unto itself in the dynamics of the model. But still, it exists.

The way that surfaces are conceived and modeled in the OL manner is by supposing an essential similarity between the bulk and the surface, and consequently conceiving and modeling surfaces as essentially like the conception and modeling of the bulk. This is an instance of a complementary phenomenon to a kind of conceptual export that has been identified by a number of contemporary philosophers of science. Hasok Chang [11, ch. 3] has called the conceptual export "semantic extension," and Mark Wilson refers to it as "property dragging," [42, ch. 6]. In the OL conception of surfaces, it is a similarity, rather than a difference, of context that licenses the application of bulk concepts like depth and volume to surface models. For the sake of brevity, I will refer to this complement to conceptual export as "property retention."

Retaining the property of depth in the OL conception of surfaces both impels and constrains the means by which OL surfaces are modeled as alike to the bulk matter they are enclosing. Again, properties and behaviors ascribed to the bulk are retained in the surface model. In the OL conception, the outermost layer is essentially similar the rest of the material; it just happens to be on the edge of the material. The retention of depth allows the surface to be modeled using concepts and interactions borrowed from the model

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of the bulk material, such as how the spatial relations in the TSK model are akin to spatial relations in bulk crystal structure.

The OL conception of surfaces underwrites the development of structural models of surfaces. For instance, Langmuir writes of his adsorption model, “The theory of surface tension which I developed . . . furnishes striking proof that the surface layers in pure liquids are normally of the thickness of a single molecule, and that these molecules are orientated in definite ways.” [24, p. 1364] This passage’s reference to thickness cannot be anything other than depth ascribed to a surface. In context, Langmuir is presenting his theory in contrast with earlier adsorption theories that supposed chemical interaction between adsorbed species and all atoms in a material, and so his remark should be read as a conclusion that adsorbates interact primarily or solely with the outermost monolayer, as opposed to with the full extent of the adsorbing material. This passage is, in effect, defining the part of the material relevant to adsorption as the outermost layer of the material. What results is an understanding of the surface that retains most of the conceptual baggage of the bulk, such that Langmuir’s model includes volume terms.

Like models of bulk materials in chemistry, too, Langmuir’s model and the TSK model both retain notions of structural decomposition. The surfaces in these models have parts that interact, as bulk materials in chemistry do. The adsorption sites in the Langmuir model are localized, as chemical bonding is, and a given site may have properties (viz. occupancy) that are either like or unlike its neighbors. The structural decomposition of surfaces in structural models does not come directly from the OL conception per se, but is ushered into the fold as a consequence of property retention from chemical models.

5.3 Parametric Models of Surfaces

Not all models of surfaces are structural. Many modeling strategies treat the surface of a system as a reduced-dimension boundary on that system. Such models either parameterize surface interactions, ignore them entirely, or cordon off surface behavior into a separate dynamical model that is later recombined with the model of bulk behavior through multiscale modeling. I shall call models of this type “parametric models of surfaces.”

In parametric models of material surfaces, three-dimensional objects are ascribed two-dimensional boundaries; two-dimensional objects are ascribed one-dimensional boundaries; and one-dimensional objects are are ascribed zero-dimensional boundaries. This approach allows researchers to study certain varieties of interaction between an object and its environment that are simply unavailable to models that treat surfaces as even very small extended regions of the same dimensionality as the objects they enclose. To take a toy example, in the classic high-school physics experiment of predicting the speed of a block sliding down an inclined plane, the region of contact between the block’s surface and the plane’s surface is modeled as a dimensionless coefficient (the friction coefficient), rather than as a spatial region of the system.

A more robust example of parametric modeling of surfaces comes from acoustics. In

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acoustics, one may model the ends of a vibrating string as zero-dimensional boundary points enclosing a one-dimensional line. Musical notes are generated by resonant (standing) sound waves. At the very outset of a note, the moment when a violinist begins to draw her bow across the string, a variety of waves propagate down the length of the string. Only certain of these waves become resonant and persist through the length of the note; the rest meet with destructive interference or dissipation in the first milliseconds of the note. The length of the string dictates what pitches persist: the string can only host standing waves whose frequencies divide evenly into the length of the string. Resonant frequencies are generated by wavelengths twice as long as the length of the string, the same length as the string, half the length of the string, $\frac{1}{3}$ the length of the string, etc. The lowest-frequency resonant frequency is known as the fundamental frequency; other resonant frequencies are known as the harmonics of the note. The complex texture of the musical note — what distinguishes its plaintive or joyous tone from the digital drone of a single-frequency sound wave — arises from the combination of fundamental and harmonic tones particular to the individual note (among other factors).

In order to explain how a given frequency is resonant for a certain length of string, and what the relationship is between the fundamental and harmonic tones of a given note, acousticians model the vibrations of the string that generate the sound wave. In these models, it is strictly necessary to model the endpoints of the string as zero-dimensional points. When a wave propagating down a string encounters the zero-dimensional boundary of the string's endpoint, acoustics models the encounter as an elastic collision in which the wave is perfectly reflected back into the string. Any spatial extension of the string's endpoint would impact the reflection of the wave, dissipating some of the wave's energy and creating a region in which, during the spatial extent of the collision, the wave would destructively interfere with itself. This would then impede the wave from achieving resonance as a persistent, standing wave in the string.[3]

For simplicity, I have given this example with a one-dimensional string enclosed by a zero-dimensional boundary, but the approach generalizes for two- and three-dimensional bodies. Importantly, even in the highly idealized, simplified case of the vibrating string, the surface in question is not a mere mathematical object; it remains a model *of a material surface*, in the sense defined in the introduction. The surfaces of the acoustic bodies in question are modeled as part of the enclosing bodies: they derive their properties, such as shape or location in space, from the shape of the body, and they impact the body in a way distinct from the impact of the environment. These surfaces enclose the materials they surround, and the acoustic phenomena they model occur at a material (cf. electron) scale.

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[3] In mathematical modeling of vibrating strings, the fixed endpoints of the string are represented as boundary conditions on the string. Bursten [7] offers a discussion of how the representation of endpoints as boundary conditions has larger ramifications for contemporary conversations about the nature of scientific explanation, as well as modeling.

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5.4 The Boundary on a Body Conception of Surfaces

The OL conception of surfaces cannot encapsulate the relevant features of a surface that are being employed in the acoustic and flow models. The OL conception's retention of depth is exactly what must be eliminated from the conception of a surface employed in such models. Instead, the conception of surface underwriting the parametric approach to modeling surfaces is the conception of a surface as a boundary on a body (hereafter the BB conception of surfaces). The BB conception is precisely the second Cartesian conception of a surface, in which "all its depth is denied." Further, the denial of depth is the feature of this conception that licenses the parameterization or reduced-dimension representation in the first place. This was illustrated in the discussion above of the need for depth to be denied to the bounding surfaces of acoustic bodies in order for resonance to arise.

The BB conception of a surface is intimately tied to the parametric approach to modeling surfaces. When a surface is conceived of as a boundary, rather than an outer later, there is no expectation of property retention of the sort seen in the OL conception's modeling strategies. In the BB conception, models of surfaces are not expected to be analogous to models of the bulk; the bulk has a depth denied to the surface, and so they are essentially — physically, mathematically — distinct.

Further, because the spatial extent of the surface in the BB conception is strictly negligible in comparison with the spatial extent of the body it encloses, it should be expected that the behavior of the bulk body makes the greater contribution to the overall behavior of the system. Parameterization is an effective modeling strategy precisely when there is a relatively smaller or less important contribution from one dynamical system than another. In this way, it may be understood how the BB conception of a surface licenses the parametric approach to modeling surfaces.

This point might be emphasized through an analogy to Nancy Cartwright's notion of a nomological machine [8, 9]. Cartwright's machines are defined as arrangements of the components and settings of a system such that it is appropriate to expect a law to occur. The view Cartwright develops excludes most of the natural world from this class of arrangements, and she argues that we can really only expect laws of nature to unfold in very particular, and usually artificially generated, contexts. In the parametric approach to modeling surfaces, the detailed behavior of surfaces is being parameterized away in order to arrange the pieces of model in such a way that a clearer understanding of internal or bulk behavior can be obtained. The treatment of surfaces in such a model is akin to arranging the components and settings of the modeled system as a "bulk-behavior machine," if you will.

Above, the OL conception of surfaces was shown to be associated with the structural approach to modeling surfaces, which was in turn shown to be characteristic of chemical considerations and methods. By contrast, the BB conception is here associated with the parametric approach to modeling. The models considered in this approach are physical more often than they are chemical. These disciplinary affiliations are not meant to be hard

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and fast, but it is worth noting them as indicators of the persistence of two conceptions of a surface.

6 From the Bending of Tiny Beams to the Problem of Conceptualizing Surfaces as Boundaries

In the BB conception of surfaces, the surface of a material lacks depth, and so constitutes a strictly negligible proportion of the matter in the material. Across parametric models of surface behavior, surface effects are modeled in a reduced dimension, relative to the the bodies they enclose. In each of the parametric cases considered above, from high-school models of friction and the acoustic models to the derivation of the boundary layer equations, what licenses the use of the surface model in question is that whatever behavior is occurring on the surface is not contributing significantly to the overall behavior of the bulk material, because the surface occupies a negligible proportion of the material's bulk.

This is exactly the assumption that breaks down at the nanoscale. The material surfaces of nanomaterials simply are not negligible boundaries. The dramatic curve in Figure 1 demonstrates just how different the proportionality is between the surfaces of nanoscale materials and their enclosing bodies, relative to the surfaces of macroscopic materials. This difference raises the question of whether and to what extent the BB conception of a surface continues to apply to nanoscale surfaces. For certain modeling scenarios in nanoscience and nanotechnology, the BB conception of surfaces may continue to prove useful, particularly in thin-film research where a nanoscale film coating is being studied for flow or transport properties. However, there is an important sense in which the BB conception of a surface simply breaks down at the nanoscale. This limits the concept of what a surface is at the nanoscale to the OL conception of surfaces, which in turn impacts nanoscale materials modeling. Indeed, the BB conception and its associated implication of a parametric modeling strategy can stand in the way of successful modeling of nanomaterials. The following case study illustrates this point. It relates an experiment that occurred in [laboratory identity blinded for review], which is still under way. As such, the case study draws not from published research, but from my observations at laboratory meetings.

The experiment in question had a simple goal: to bend silver nanorods. Unlike macroscopic rods of silver, silver nanorods are too small to be grasped by nano-tweezers and simply tugged at each end. Instead, an elaborate chemical process was devised to induce a bend on the nanorods. This process began with a silver acid in solution. A multi-step chemical reaction then precipitated the rods out of the acid solution, and another to stopped them from growing above a certain size. Both these reactions required highly controlled conditions and careful measurement and timing. The protocol continues with the synthesis of small spherical beads of silicon in a distinct chemical environment. These beads were synthesized to be significantly larger than the rods, so that the rods could stick to their sides without bending. The beads were then coated in one kind of chemical

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(avidin) and the rods in another (biotin). The two coatings are naturally attracted to one another, which caused the rods to stick to the beads once the two solutions were mixed. In the final stage of the experiment, an additional agent was introduced into the solution to shrink the silicon beads, generating a bend in the rod stuck to the bead as the curvature beneath it changes.

Clearly, the experimental protocol was complex and fraught with potential for error, so it was no surprise when at first the experiment did not succeed. However, after a number of trials and adjustments in the recipe, the experiment was still systematically failing. Ultimately, it was discovered that the reason for the failure was not due to the experimental design. Rather, it was a problem in the mathematical models being used to generate the proportions of materials needed for the synthetic protocol. Specifically, the breakdown was occurring in the calculations of the force required to bend the rods. In the models being used, the force required to bend the rods was modeled using the Young's modulus of silver. Young's modulus is a property of materials that is defined within continuum-mechanical models of materials and which measures bulk behaviors. Models that employ Young's modulus typically ignore surface effects entirely in the consideration of elastic deformation. In macroscopic materials, this strategy works well because surfaces make up a negligible proportion of the overall material, so differences in mechanical behavior between the bulk and the surface may be ignored; this is the tacit assumption in parametric models. The problem was that the silver nanorods in the experiment did not have a negligible proportion of their material on their surfaces; like most nanomaterials, the surface occupied a significant proportion of the material and was, consequently, responsible for a greater proportion of the rods' overall mechanical behavior. The experimenters changed their modeling approach to one that modeled the rods' bending via surface restructuring (a structural model similar to the TSK model), and the experiment has enjoyed greater success as a result.

In this experiment, conceiving of the surfaces of the nanorods as boundaries on bodies interfered with experimental design and outcome by steering the experimenters toward inappropriate modeling strategies. Switching the conception of surfaces led to a change in the modeling choices made, and eventually to an experimental protocol that succeeded where the previous ones had failed. This case illustrates two points, which I wish to emphasize. First, how surfaces are conceived of matters, not just for philosophical idling, but for the design and carrying out of experiments. This experiment is not an isolated case; throughout nanoscience, researchers wrestle with how to model the materials they are making, and in these struggles they regularly encounter questions of how to think about the surfaces of the materials they make. Second, due to the proportionality difference, the BB conception of surfaces is far less applicable to nanomaterials than it is to macroscopic materials, and as such researchers should exercise caution when deploying parametric models of surfaces in nanoscience.

One consequence of this difference is mereological: There is an important sense in which the surface of a nanomaterial is not the same part of the material as the surface of a bulk

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material. Nanomaterial surfaces contribute to the mass and volume of the materials they enclose. They also contribute significantly to the properties and behaviors of nanomaterials. This change in surfaces at the nanoscale also demonstrates the separability of the two conceptions of surface discussed above. The OL conception and the BB conception come apart at the nanoscale, and the BB conception begins to break down. To put the point another way, at such a small scale (indeed, the smallest scale to which the notion of a material surface can apply), the notion of a surface has not yet realized all its conceptual potential.

Wilson has introduced the notion of "conceptual directivity" as an alternative to historical analytic technical vocabularies such as "intension" and "denotation." [42, p.15] In Wilson's view, the directivity of a predicate or a concept (he discusses both at length and applies the term to each) is a complex and historically contingent encapsulation of the operational, linguistic, mathematical, and conceptual associations between a given concept and other nearby ones, which are collectively aimed at determining whether a concept or predicate has been rightly applied in a particular use case. This idea can be useful in diagnosing what I believe has happened to the concept of a surface at the nanoscale: the concept of a surface has not acquired all of, and has shed some of, the directivities that will come to be associated with it upon arrival at the nanoscale. The associations and inferences that can come from thinking about a surface *as a boundary on a body* are much less reliable at the nanoscale than they are in macroscopic materials modeling, and so they do not comprise part of the directivity of the application of surface concepts to nanoscale materials modeling; conversely, the novel and scale-dependent properties and behaviors of nanoscale surfaces are not captured in their entirety by the directivity of either the OL or the BB conceptions. This latter point suggests that we should expect to see entirely new modeling strategies developed to understand nanoscale surfaces, which has indeed come to pass.

One consequence of the shifting directivity of the concept of a surface at the nanoscale is that once surfaces are no longer mere boundary regions, surface behaviors are no longer mere boundary behaviors. As surfaces shed their negligible-boundary associations of the BB conception, surface behaviors come to be, in some cases, the dominant or primary behavior of a material. One way of conceptualizing this change is to think of the interior, or bulk, behavior region shrinking relative to the region of surface behavior, so that, in some cases, it is the bulk behavior that can be idealized away as a mere "boundary" effect.[4]

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[4] I have framed this discussion in terms of concepts and modeling strategies, but it is not difficult to see an extension of what has been said here into the domain of scientific metaphysics. In such an extension, I believe the results of this discussion would be usefully put into conversation with Ladyman's [22, p. 152] requirement that scientific ontologies be "scale-relative." The scale-dependent, or scale-relative, shedding and acquisition of conceptual associations suggests that surfaces are simply not the same thing at the nanoscale as they are at the macroscale, and as such, that "nanoscale surface" and "macroscopic surface" occupy distinct regions of ontological space in a way that agrees with Ladyman's view. However, it is not clear to me how the conceptual throughline of the OL notion of a surface, which is shared through the ontological splitting, is accommodated in Ladyman's account. I hope to pursue this puzzle at more length

7 Conclusions: Easing the Tension

One upshot of recognizing the distinction between the two conceptions of surface used in contemporary scientific modeling is that, in many instances, physics and chemistry are simply talking about different things when it comes to modeling surfaces. Most of the time, this is no cause for concern, as the tent of scientific modeling is large, and there is room for many approaches inside it. However, the ships-in-the-night quality of this contrast gives rise to both a philosophical and a practical challenge. Philosophically, even a mild preference for conceptual clarity could lead one to ask which of the two conceptions of a surface is more fundamental, whether one conception reduces to the other, or whether there are at the very least clear lines between contexts in which one or the other conception is at play. Practically, it happens to be the case that there are instances of contemporary scientific modeling where both conceptions are employed in the construction of a single scientific model, and when these instances arise, some account is warranted of why such models should be trusted. Even if the philosophical challenge is not satisfactorily resolved, the conception of surface being employed will impact the modeling choices made and thus the rationale for trusting, believing in, or otherwise obtaining information from, the models. In this section I conclude the present discussion by arguing for a particular sort of contextual account of the concept of a surface, specifically one in which changes in scale signal shifts in conception and constrain changes in modeling strategy.

First, the philosophical challenge, namely the question of whether one of the two conceptions of surface is more fundamental than the other. On the face of it, this challenge does not have an intuitive or obvious answer. There is simply no middle ground between having and lacking depth, and one is not a special case of the other. Traditional reductionist approaches to resolving fundamentality issues typically suggest reducing chemical approaches to physical ones, rather than the other way around; in this case, that would imply that the BB conception is "more fundamental." However, the OL conception is more commonly associated with micro-scale representations of surfaces, in that it OL models contain dynamics of parts that the BB models lack. Similarly, the BB conception treats surfaces as inherently depth-less, which may strike some as an idealization that the more fundamental conception should be able to de-idealize.

Conceiving of the surfaces of three-dimensional bodies as three-dimensional rationalizes the retention of properties from the bulk of a material in the structural modeling of its surface. It also generates the conditions necessary to develop a conception of the surface as having additional structure, beyond its mere depth. This structure generates internal differences among pieces or parts of a surface, such as the bonding sites in the TSK model and the notion of occupancy in the Langmuir model. These phenomena are what the models are about; they are the central behaviors being studied by the models, not mere byproducts of mathematical or representational necessity. When a surface is conceived as a

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someday.

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boundary on a body, there is no room for such internal structure to manifest. Consequently, the sorts of things that OL models are about cannot be redrawn in BB models.

Faced with these limits, another potential resolution could be via a contextual route, that is, simply to treat the notion of a surface as context-sensitive and to index different conceptions to different modeling contexts. Resolving conceptual conflict via indexing a concept to a context has been suggested many times before for assorted scientific concepts of interest, from the identity between water and H_2O [25], the question of what constitutes boiling [11], and the notion of hardness [42]. In her monograph on substance concepts, Millikan [28] develops a similar theme from a different philosophical tradition, drawing on analytic philosophy's tradition of analysis of the concept of a concept. Her view argues that conceptions of a substance are inherently contextual, although her account of the concept underlying such conceptions is much more complex and nuanced. Indeed, the very idea of a contextual resolution to understanding the concept of a surface is inherited from the long arm of analytic philosophy, dating back at least to Frege's modes of presentation. Under such a resolution, one would simply separate the chemical settings from the physical, or perhaps the structural contexts from the parametric.

Wilson's account of concepts offers its own vocabulary for context-sensitive applications of concepts. He uses the term "conceptual multi-valuedness," [42, ch.6] to emphasize how differences in the environment in which a piece of conceptual architecture is embedded can influence the network of associations it invokes. In deconstructing concepts such as hardness and weight, Wilson demonstrates that features of the material, of the testing apparatus, and of the employer of the term each contribute to how a term are used in any given setting. What it takes to call a piece of steel "hard" for the purposes of determining its suitability as a piece of rebar for a given construction project is simply different than what it takes to call a piece of wood "hard" when considering it for use as a cutting board. Wilson suggests that understanding how we employ concepts, such as hardness, is a matter of bringing into view the rough-edged patchwork of associations that span the gaps between these varied uses.

This account can assist in moving the conversation from the fundamentality problem to the more general problem of how modeling practices should incorporate the two concepts of a surface. Wilson's account employs a richer and more nuanced set of suggestions than simply indexing a particular conception to a given context, and much of his view arises from extended discussions of exactly how gaps are spanned between distinct uses of a given concept across theoretical contexts. Thinking of *surface* as a multi-valued concept does capture some of the complexities discussed so far. However, it does not explain why the two conceptions come apart in the first place, nor why the decoupling happens where it does. Neither does it offer any sort of prescription for how to respond to it. To address these issues, it is necessary to see the concept of a surface not just as multi-valued, but as scale-dependent. The very scale at which the conceptions come apart drives them to separate. At this scale, the shape of the game for materials has changed. The two notions of surface come apart at the nanoscale because that is the scale where the material itself

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is only ever so slightly larger than its atomic components, where the outermost layer of atoms in a material is something more substantial than a negligible boundary (here again is a blurring of the models-to-metaphysics line discussed in Footnote 6). As the scale of a material changes, so do the conceptual resources we have on hand to describe its parts, its challenges, and its behaviors. Resolving the decoupling of the two conceptions of surface at the nanoscale is a matter of realizing that the scale itself has generated a shift in the meaning of the concept: *surface* is a scale-dependent concept.

There are a number of common enough modeling contexts outside nanoscience in which there is still not a simple choice to be made between conceptions. These can include instances where a material is being studied for both properties of chemical interest and properties of physical interest, such as a copper wire being tested simultaneously for electrical resistance and resistance to corrosion. In the development of lubricants for engineered materials, similarly, there is a need to model both parameterized frictional forces (e.g. to determine the degree to which a particular formulation reduces friction) and structural interactions (e.g. chemical reactions between a particular formulation and the surfaces it lubricates). In these cases, as in the boundary-layer case in Section 3, it is apparent that it is not *mere* context that resolves the apparent contradiction between the two conceptions, but rather a particular sort of context, namely, the scale of resolution that the model aims to represent. While the nanomaterials case makes it clear just how large a role scale can play in guiding the directivities of the surface concepts used to construct scientific models, scale is still at play even in macroscopic materials modeling contexts.

The central goal of this article has been to show that the notion of a surface as it is employed in contemporary materials modeling is far from straightforward, and that its complexities generate concerns for philosophers as well as for scientific modelers. In the course of arriving at a greater understanding of the notion of a surface, I have also lately advocated a scale-dependent account of scientific modeling. In particular, the irreducibility of one type of surface model to another offers evidence against a reductive approach to modeling surfaces. Further, the scale-separation of surface models in boundary layer modeling, as well as the breakdown of the BB conception of surfaces at the nanoscale, suggest a greater role for scale in the epistemology of modeling. In fact, it seems likely that scale plays a significant and wide-ranging role in conceptual activities across the physical and life sciences. Some recent accounts of inter-theoretic relations, especially those focused on the physical sciences, have advocated replacing the vocabulary of "levels" with that of scales or suggested that that scale separation, rather than fundamentality, is a distinguishing factor between physical theories (e.g. [1, 35, 2, 22, 39]; see also [38, 36]). The results of this project align with those suggestions. Investigating how scale figures into scientific reasoning more broadly has the potential to reshape philosophical understanding of scientific modeling and conceptualizing, just as investigating nanoscale phenomena has reshaped scientific understanding of material behavior.

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