What Is Nanotechnology and Why Does It Matter?

From Science to Ethics

Fritz Allhoff, Patrick Lin, and Daniel Moore

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Preface

New and emerging technologies both excite and worry us – academics, policymakers, businesses, investors, ethicists, journalists, futurists, humanitarians, the global public – and nanotechnology today is certainly a flashpoint for irrational exuberance and fears. By definition, there is a knowledge gap during the nascent stages of any new technology, and nanotechnology is no exception: researchers and engineers are still learning about nanoscience and its applications. But, in the meantime, hope and hype naturally and irresistibly fill this vacuum of information.

In nanotechnology, we find an entire range of speculative possibilities, from limitless life to the end of days. Depending on whom you ask, nanotechnology is predicted to help solve the world's energy and hunger issues. Or it can help us easily ride into orbit on a space elevator or evolve into cybernetic beings. Or by playing with this fire – by manipulating the basic building blocks of nature – nanotechnology may scorch the earth and fulfill a prophecy of Armageddon. We may finally cause our own undoing by unleashing a powerful technology that we do not yet fully understand and thus may not be able to control.[1]

So which is it: will nanotechnology usher in a bright era for humanity, or its reckless demise? Or perhaps neither: nanotechnology could be much ado about nothing, given the admittedly humdrum products it enables today from longer-lasting tennis balls to stain-resistant pants. Of course, none of us knows the answer, despite a continuous flood of predictions. But what

[1] In addition to forthcoming discussion in this book, see Fritz Allhoff, Patrick Lin, James Moor, and John Weckert (eds), *Nanoethics: The Social and Ethical Implications of Nanotechnology* (Hoboken, NJ: John Wiley & Sons, 2007). See also Fritz Allhoff and Patrick Lin (eds), *Nanotechnology and Society: Current and Emerging Ethical Issues* (Dordrecht: Springer, 2008).

we do know is that nanotechnology is rapidly entering the marketplace today, and ongoing research reveals risks (e.g., environmental and health harms) as well as fantastical innovations (e.g., invisibility cloaks and 'smart dust'). It is also becoming clear that nanotechnology has the potential to profoundly change the world, even if today's products are uninspired and only incrementally better than previous ones. Therefore, understanding what nanotechnology is and why it matters is the first step in a roadmap toward our future: it is the next generation for industries, financial markets, research labs, headlines, and our everyday lives.

In this book, we hope to tame the riot of speculation with an informed and balanced look at nanotechnology and its issues. To that end, this book is organized in three units. First, we discuss the science behind nanotechnology, including the nanoscale, tools of the trade, nanomaterials, and applied nanotechnology. In the second unit, we provide a general framework to evaluate the particular ethical and social issues that nanotechnology raises (which are then covered in the third unit); for instance, we will discuss the different ways to understand risk, regulation, and fairness in the use and dissemination of nanotechnology. In the third unit, we dedicate chapters to some of the most urgent and contentious applications of nanotechnology: environment, military, privacy, medicine, and enhancement. In choosing this list, we have focused on near- and mid-term issues rather than more speculative ones – such as life extension, space exploration, and molecular manufacturing – though these latter are mentioned when appropriate. We should also note that given the unusually broad range of issues that arise in connection with the social and ethical implications of nanotechnology, we have made specific choices regarding our coverage; to this end, we have focused on core scientific and philosophical issues and ones on which we are qualified to write. Other important topics – such as existing (and potential) laws and regulations, economic impacts, and so on – can be pursued elsewhere by the interested reader.

While all of the chapters were the result of collaboration, one or other of us bore the primary responsibility for each. Having one scientist and two philosophers on the project undoubtedly makes it stronger and, while our disciplinary backgrounds undoubtedly come through, we hope the presentation and styles are well integrated; editing a project like this takes as long as writing it! Some of the chapters have extended scientific or philosophical primers, which we include for those with less background and/or for pedagogical reasons as this book stands for various course adoptions. Those with the relevant professional training can certainly skip these discussions.

New technologies are not easy to understand, nor are the public policy questions they engender. Therefore, we commend you, the reader, not only for your patience in sorting through these issues, but also for your foresight in recognizing how essential nanotechnology will be to society and our collective futures.

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Unit I

What Is Nanotechnology?

1

The Basics of Nanotechnology

1.1 Definitions and Scales

Before delving into the depths of nanotechnology and nanoscale science, we should be clear what we mean when we use terms such as 'nanotechnology,' 'nanoscience,' and 'nanoscale.' It is a basic nomenclature, used to describe certain attributes of certain systems, and such nomenclatures are typically designed to eliminate confusion and encourage accurate communication among those discussing the system. To be sure, there will be several other variants of words with the prefix 'nano-' used in this book and it is important to make sure that we have our meanings straight if any sort of meaningful discussion is possible.

The prefix 'nano-' is derived from the Greek word *nannos*, meaning "very short man." Most of the measurement prefixes used today originate from Greek and Latin words used in measurements. For example, 'kilo-' is from the Greek word *khilioi* meaning "one thousand" and 'milli-' is from the Latin word *mille* meaning "one thousand." Greek and Latin words for numbers cover the everyday level of measurements from one-thousandth to one thousand. Beyond that, it gets interesting. To describe one billion (1,000,000,000) of something we use the prefix 'giga-' which is from the Greek word *gigas* meaning "giant." We also get the word "gigantic" from this root. On the other end of the spectrum, to describe one millionth (0.000 001) we use the prefix 'micro-' from the Greek word *mikros* meaning "small." To describe one trillionth (0.000 000 000 001) we use the prefix 'pico-' from the Spanish word *pico*, which can mean both a "beak" and a "small quantity." These prefixes are extremely useful when discussing very large or very small values. For example, we could refer to the radius of the Earth at its equator as being 6,378,100 meters, but it is more useful (and requires less effort) to refer to it as 6,378.1 kilometers. The most common scientific prefixes and their derivations are shown in Table 1.1.

Table 1.1 Etymology of scientific prefixes

Prefix	*Language of origin*	*Word*	*Meaning of word*	*Value*
Zetta	Latin	Septem	Seven	$(10^3)^7 = 10^{21}$
Exa	Greek	Hexa	Six	$(10^3)^6 = 10^{18}$
Peta	Greek	Penta	Five	$(10^3)^5 = 10^{15}$
Tera	Greek	Teras	Monster	10^{12}
Giga	Greek	Gigas	Giant	10^9
Mega	Greek	Megas	Great	10^6
Kilo	Greek	Khilioi	One thousand	10^3
Hecto	Greek	Hekaton	One hundred	10^2
Deca	Greek	Deka	Ten	10^1
Deci	Latin	Decem	Ten	10^{-1}
Centi	Latin	Centum	One hundred	10^{-2}
Milli	Latin	Mille	One thousand	10^{-3}
Micro	Greek	Mikros	Small	10^{-6}
Nano	Greek	Nannos	Dwarf	10^{-9}
Pico	Spanish	Pico	Beak, small quantity	10^{-12}
Femto	Danish	Femten	Fifteen	10^{-15}
Atto	Danish	Atten	Eighteen	10^{-18}
Zepto	Latin	Septem	Seven	$(10^{-3})^7 = 10^{-21}$

At its root, the prefix 'nano-' refers to a scale of size in the metric system. 'Nano' is used in scientific units to denote one-billionth (0.000 000 001) of the base unit. For example, it takes one billion nanoseconds to make a second. In everyday practical use, the term 'nanosecond' is not very useful in describing time accurately. Imagine discussing time in these terms: we would say things like "dinner will be ready in 300,000,000,000 nanoseconds." Instead, the term 'nanosecond' is mainly used to refer to a very short period of time. (A nanosecond is to a second as one second is to approximately 30 years.)

When we are talking about *nano*technology, we are talking about a scale – an order of magnitude – of size, or length. We are making a reference to objects that are sized on a scale that is relevant when we discuss *nanometers* (nm). Using this terminology makes it easier to discuss the size of objects that are the main attraction in nanotechnology, namely atoms. If we were to describe the size of atoms and molecules in feet or meters, we would have to say that a hydrogen atom (the smallest atom) is 7.874×10^{-10} feet or 2.4×10^{-10} meters. Instead, we can use nanometers and say that the hydrogen atom is 0.24 nm.

The nanoscale, then, is the size scale at which nanotechnology operates. Though we have a lower limit on this scale size (the size of one atom), pinning down an upper limit on this scale is more difficult. A useful and well-accepted convention is that for something to exist on the nanoscale, at least one of its dimensions (height, width, or depth) must be less than about 100 nanometers. In fact, it is these limits to the nanoscale that the National Nanotechnology Initiative (NNI) uses for its definition of nanotechnology: "Nanotechnology is the understanding and control of matter at dimensions of roughly 1 to 100 nm, where unique phenomena enable novel applications."[1] To this, it is useful to add two other statements to form a complete definition. First, nanotechnology includes the forming and use of materials, structures, devices, and systems that have unique properties because of their small size. Also, nanotechnology includes the technologies that enable the control of materials at the nanoscale.

Though we have established that the 'nano-' in 'nanotechnology' signifies a particular scale, it is important to get a good idea of what that scale is – that is, what size the nanoscale is in relation to our everyday experience. There are several analogies that we can use to explain the size of a nanometer in relation to sizes that are more commonly known. For example, it takes 50,000 nm to make up the width of a single strand of human hair. Another example is as follows: a nanometer compared to the size of a meter is roughly of the same proportion as a golf ball compared to the size of the Earth. Perhaps the best way to illustrate the nanometer scale is by describing the range of length scales from the centimeter down to the nanoscale. An ant is on the order of 5 mm (10^{-3} meters) in size. The head of a pin is 1–2 mm. A dust mite is 200 μm (10^{-6} meters) in size. A human hair is about half the size of a dust mite, 100 μm wide. The red blood cells that flow in our veins are about 8 μm in diameter. Even smaller than that, the ATP synthase of our cells is 10 nm (10^{-9}) in diameter. The size of the double helix of DNA on the nanoscale is about 2 nm wide. Finally, atoms themselves are typically less than a nanometer in size and are sometimes spoken about in terms of angstroms (10^{-10} meters).

1.2 The Origins of Nanotechnology

Nanotechnology, like any other successful technology, has many founders. In one sense, the very field of chemistry has been working on nanotechnology since its inception, as have materials science, condensed physics, and solid state physics. The nanoscale is not really all that new. But investigating and designing with a specific eye on the nanoscale is new – and revolutionary.

The term 'nanotechnology' can be traced back to 1974. It was first used by Norio Taniguchi in a paper entitled "On the Basic Concept of 'Nano-Technology'."[2] In this paper, Taniguchi described nanotechnology as

[1] "What is Nanotechnology?" National Nanotechnology Initiative. Available at http://www.nano.gov/html/facts/whatIsNano.html (accessed October 11, 2008).

[2] Norio Taniguchi, "On the Basic Concept of Nanotechnology," *Proceedings of the International Conference of Production Engineering, London, Part II*. British Society of Precision Engineering, 1974.

the technology that engineers materials at the nanometer level. However, nanotechnology's history predates this. Traditionally, the origins of nanotechnology are traced back to a speech given by Richard Feynman at the California Institute of Technology in December 1959 called "There's Plenty of Room at the Bottom."[3] In this talk, Feynman spoke about the principles of miniaturization and atomic-level precision and how these concepts do not violate any known law of physics. He proposed that it was possible to build a surgical nanoscale robot by developing quarter-scale manipulator hands that would build quarter-scale machine tools analogous to those found in machine shops, continuing until the nanoscale is reached, eight iterations later. As we will see, this is not exactly the path that nanotechnology research has actually followed.

Feynman also discussed systems in nature that achieve atomic-level precision unaided by human design. Furthermore, he laid out some precise steps that might need to be taken in order to begin work in this uncharted field.[4] These included the development of more powerful electron microscopes, key tools in viewing the very small. He also discussed the need for more fundamental discovery in biology and biochemistry. Feynman concluded this talk with a prize challenge. The first challenge was to take "the information on the page of a book and put it on an area 1/25,000 smaller in linear scale, in such a manner that it can be read by an electron microscope."[5] The second challenge was to make "an operating electric motor – a rotary electric motor which can be controlled from the outside and, not counting the lead-in wires, is only 1/64 inch cube."[6] He ended the talk by saying "I do not expect that such prizes will have to wait very long for claimants."[7] He was right about one of the prizes: the motor was built fairly quickly and by a craftsman using tools available at the time. However, it was not until 1985 that a graduate student at Stanford named Tom Newman reduced the first paragraph of Charles Dickens' *A Tale of Two Cities* to 1/25,000 its size.

In his paper on the basic concept of nanotechnology, Taniguchi developed Feynman's ideas in more detail. Taniguchi stated, " 'Nano-technology' is the production technology to get the extra high accuracy and ultra fine dimensions, i.e., the preciseness and fineness of the order of 1 nm

[3] Richard P. Feynman, "There's Plenty of Room at the Bottom," *Journal of Microelectromechanical Systems* 1 (1992): 60–6.

[4] Physicists, especially, had not explored this field much. Most physicists at the time were focused on high-energy physics, probing into the atom to look at quarks and subnuclear reactions, astrophysics, or nuclear physics. Much of what fell in between was left to chemists and engineers, as many of the fundamental equations in this area of the natural world were believed to be explained already.

[5] Feynman, "There's Plenty of Room," p. 66.

[6] Ibid.

[7] Ibid.

(nanometer), 10^{-9} m in length. With materials the smallest bit size of stock removal, flow, or design is one atom (generally about 1/5th of a nanometer), so the limit of fineness of materials is on the order of one nanometer."[8] In the paper, Taniguchi discussed his concept of 'nanotechnology' in materials processing, basing this on the microscopic behavior of materials. Taniguchi imagined that ion sputtering would be the most promising process for the technology. As we will discuss later in this section, many tools and techniques are used for the development of this type of nanotechnology.

Then, in 1987, K. Eric Drexler published his book, *Engines of Creation: The Coming Era of Nanotechnology*.[9] Aimed at a non-technical audience while also appealing to scientists, Drexler's book was a highly original work describing a new form of technology based on molecular "assemblers," which would be able to "place atoms in almost any reasonable arrangement" and thereby allow the formation of "almost anything the laws of nature allow." This may sound like a fanciful and fantastical idea but, as Drexler points out, this is something that nature already does, unaided by human design, with the biologically based machines inside our own bodies (and those of any biological species). There has been significant debate about the possibilities, promise, and troubles with what is now called "molecular manufacturing." Even the possibility of these machines is widely debated. Suffice it to say, however, that *Engines of Creation* marks a distinct jumping-off point for nanotechnology and the associative scientific research. Even though much of this research had nothing at all to do with molecular manufacturing, the focus on the scale of the research objects became the most important factor. Tools developed to handle individual atoms, such as the scanning probe microscope at IBM, enabled researchers to study and manipulate individual atoms and molecules with a degree never before possible. In a very famous image, researchers at IBM moved xenon atoms around on a nickel substrate with a scanning tunneling microscope. This image used the atoms to spell out the company's logo, "IBM." Electron microscopes developed to the point that they could be in more and more research environments (including, sometimes, in biological applications as Feynman desired). Able to see individual atoms and their arrangements within materials, researchers began to study developing atomically precise materials and devices.

The discovery of novel materials on the nanoscale notably began with the Buckminsterfullerene (also called the buckyball). The buckyball was so named because of the resemblance to the geodesic domes that the architect Richard Buckminster Fuller popularized. Discovered in 1985 at Rice University, it consists of an arrangement of 60 carbon atoms. In 1991,

8 Taniguchi, "On the Basic Concept."

9 Eric Drexler, *Engines of Creation: The Coming Era of Nanotechnology* (New York: Broadway Books, 1987).

nanoscale materials became the focus of intense research with the discovery of the carbon nanotubes by Sumio Iijima of NEC. At a somewhat feverish pace, novel nanoscale material after novel nanoscale material has been reported ever since. Nanotechnology is now recognized as the future of technological development. In 2000, the US government developed the National Nanotechnology Initiative (NNI) in order to administer funding and develop nanotechnology as the major research thrust of the twenty-first century.

1.3 The Current State of Nanotechnology

Having looked at the basic history of nanotechnology, we can now investigate where we currently stand. In particular, how is nanotechnology researched in laboratories across the world today? What is the current direction of nanotechnology research? The answer helps us understand the development, characterization, and functionalization of nanoscale materials and the science that governs them. This involves three main thrusts of research: nanoscale science (or "nanoscience" – the science of interaction and behavior at the nanoscale), nanomaterials development (the actual experimental development of nanoscale materials, including their use in device applications), and modeling (computer modeling of interactions and properties of nanoscale materials).

Understanding the underlying science of nanoscale interactions is extremely important to the development of nanotechnology; these interactions constitute one of the main areas of research in the field of nanotechnology. The laws of physics that operate on objects at the nanoscale combine classical (or Newtonian) mechanics, which governs operations of everyday objects, and quantum mechanics, which governs the interactions of very small things. Though many of the fundamental laws of nature that operate on this level have been discovered, science at this scale is still very difficult. Quantum mechanics works at this scale, but the interplay between the high number – that is, greater than two – of atoms in nanoscale materials can make it difficult to predict the actual outcome of these interactions. Furthermore, classical mechanics works on this scale, but the small size of the materials and the close scale of the interactions can make forces that are well understood at large scales (e.g., friction) and/or powerful at those scales (e.g., gravity) mysterious and/or less powerful at the nanoscale. Understanding the forces and theories at play within nanotechnology is just one aspect of nanoscience.

Another very important aspect of nanoscience is understanding the formation of nanoscale materials and devices. In looking at the nanoscale, traditional (non-nano) materials, structures, and devices are often referred to as "bulk technology." To be sure, this "bulk" style of technology has led to many great accomplishments: we easily make wonderful computing devices, ultra-strong steel, and very pure ceramics. Using bulk technology, we can create exquisitely small devices and materials. However, this creation is still done by cutting, chipping, pounding, extruding, melting, and performing other such bulk procedures to materials to create the new device, structure, or material. The main difference with nanotechnology is this creation process. With nanotechnology, we start on the atomic scale and, controlling atomic/molecular placement and arrangement, we build up the technology into unique devices, materials, and structures. This new type of formation requires new types of synthesis, requiring a new understanding of the formation of materials on the nanoscale. Furthermore, many materials have extremely unique properties when they are developed at a nanoscale. Many materials configure themselves in different atomic arrangements not seen in the bulk form of the same materials. Understanding the changes that these materials undergo as they are formed on a smaller scale is vital to developing the use of these materials in devices.

Nanotechnology today focuses, as we have already mentioned, on the development, understanding, and use of materials at the nanoscale, or nanomaterials. Materials are made up by an arrangement of particular atoms – typically in a specific way – which helps define the property of the material. For example, steel is one of the strongest engineering materials, and its strength will increase as carbon is added to it. Steel is made of mostly iron with other elements added: stainless steel, for example, contains 10 percent chromium to protect the material against corrosion.

Actually, materials throughout history have basically defined the technology of the age. We refer to the Stone Age and the Iron Age because of the types of materials that were used or developed during those eras to make the technology that was used in everyday life. For example, the Bronze Age was a period in civilization's development when the most advanced widespread metalworking consisted of techniques for smelting copper and tin from naturally occurring ore and then alloying those metals in order to cast bronze. In more modern times we can see that the development of methods for using silicon and other semiconductors is essential to developing modern computing devices and many other devices that we use on a daily basis.

On the nanoscale, this association between material, device, and structure only amplifies since these are virtually indistinguishable from each other at that scale. Nanomaterials can also be used in conjunction with other materials, thus augmenting the properties of those other materials. In this sense, nanoscale materials have been important to the materials field for some time. For example, nano-sized carbon black particles have been used to reinforce tires for nearly 100 years. Another, more common, example is precipitation hardening of materials. Precipitation hardening is a heat treatment technique that is used to strengthen materials, particularly some metals. It relies on producing fine, impure nanoscale particles, which then impede the moving of defects within the material. Since these defects are the dominant cause of plasticity in materials, the treatment hardens the material. This accidental discovery in 1906 allowed for significant improvements in the strength of aluminum. At the time, researchers could not image these precipitates. It was later discovered that the precipitates were nano-sized particles.

Materials are the essence of technology at the nanoscale. Because of the scale of the technology, the atomic species and structure define not only the properties of the material but also the function of the device. Furthermore, different materials interact differently with their environment when they are sized on the nanoscale. Bulk materials interact with their environment in a certain way because the vast majority of their atoms are inside the volume of the material rather than on the surface; this makes the surface-to-volume ratio very small. Atoms respond to their environment differently when they are surrounded by other atoms than when they are on a surface and do not have atoms surrounding them. And the relative amount of atoms on the surface can greatly influence the properties of the material as a whole. With nanoscale materials, many of the atoms reside on the surface of the material and therefore the surface-to-volume ratio is much larger. For example, a spherical particle that has a radius of 100 micrometers will have a surface-to-volume ratio of about 30,000. This may seem large, but the percentage of atoms on the surface of the material is very small, only 0.006 percent (that is, only 6 out of every 100,000 atoms are on the surface). Compare this with the surface-to-volume ratio of a particle that has a radius of 10 nm. This ratio would be 300,000,000. Here, the percentage of atoms on the surface of the material is a much larger 6 percent (or 6 out of every 100). This can radically change the properties of the material, how it interacts with its environment, and how it can be used in devices.

Another important aspect of nanotechnology is the modeling of nanoscale devices, materials, and interactions. Modeling has an interesting history, through which initially scientists would build actual physical models of molecules and structures in their offices. With these models they would perform the calculations for each atom, move them around on their model, and then start the process all over again – iteration after iteration. John Desmond Bernal, a scientist who pioneered using X-rays to examine the structure of materials, was one such modeler. As he wrote: "I took a number of rubber balls and stuck them together with rods of a selection of different lengths ranging from 2.75 to 4 inch. I tried to do this in the first place as casually as possible, working in my own office, being interrupted every five minutes or so and not remembering what I had done before the interruption."[10] Clearly, another way to perform these calculations was necessary.

[10] John Desmond Bernal, "The Bakerian Lecture, 1962: The Structure of Liquids," *Proceedings of the Royal Society* 208 (1964): 299–322.

Though the simplest calculations can be done by hand on a sheet of paper, computers are required for understanding and modeling the behaviors of large systems (including biological molecules and chemical systems). For these, a massive amount of computing power is necessary. Modern modeling systems that are used in predicting the behavior of nanoscale systems all rely on the atom as their fundamental unit.[11] Modeling provides an approximate solution. The reason that an exact solution cannot be determined for many arrangements is known as the "many-body problem." This problem is best illustrated by looking at quantum mechanics. When we are trying to determine the energy of an atom, the electrons play a central role. Let us look at a few equations just to see how much more complicated they become as electrons are added; without any technical knowledge about how to solve the equations, this point should still be readily apparent. For example, if we wanted to determine the energy of a hydrogen atom (with one electron and one proton), the equation looks like this:

$$E_\alpha = \frac{<\psi_\alpha|\hat{H}|\psi_\alpha>}{(<\psi_\alpha|\psi_\alpha>)}$$

where the symbols are standard quantum mechanical symbols.[12] This problem can be solved by hand. Now, if we add an electron to the system as in a helium atom, the equation becomes more complicated:

$$\left[-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{|\overline{r_1} - \overline{r_2}|}\right]\psi(\overline{r_1}, \overline{r_2}) = E_{\text{el}}\psi(\overline{r_1}, \overline{r_2})$$

This is still solvable by hand, though it would take a little more work. Beyond this, however, the problem becomes unsolvable exactly; it has to be approximated. The equation for the many electrons looks like the following:

$$\left[-\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \frac{Z}{r_j} + \sum_i \sum_{j>i} \frac{1}{|\overline{r_i} - \overline{r_j}|}\right]\psi(\overline{r_1}, \ldots, \overline{r_n}) = E_{\text{el}}\psi(\overline{r_1}, \ldots, \overline{r_n})$$

This equation is unsolvable when the number of electrons is greater than two. The tabulation of a function of one variable requires about a page, but a full calculation of the wave function (the description) of the element

[11] This may not seem all that special, but physical and chemical law relies on quantum calculations in which the atom is not the fundamental unit. In quantum chemistry, the electron is the fundamental unit; it helps determine the bonding of the atoms and the electrical/magnetic characteristics of the material.

[12] It is not within the scope of this work, nor is it necessary to get into the details of the calculation. Rest assured that this calculation is relatively simple and can be performed by hand on the back of an envelope to receive an exact answer.

iron has 78 different variables in it. Even if we simplified the number of each variable to a number like 10 (a very crude approximation), the full determination would require 10^{78} entries. That's a one with 78 zeros after it for just one iron atom. Imagine if we want to determine the properties and interactions of more complex systems! Clearly, approximation is necessary.

Computer simulation and modeling are not without their limitations. A simulation is at best as good as any underlying assumptions. Oftentimes the assumptions and simplifications are ill-conceived, which can cause the results to be misleading. Furthermore, long simulations can be ill-conditioned (i.e., not well suited for computation) and will accumulate errors. A better choice of algorithm can help relieve this problem, but it cannot eliminate it completely. Also, many of the functions used for simplification are not very good for large systems (because of the problems mentioned earlier), and the molecular dynamics simulations that are based on them will come out flawed. Overall, the larger the system being modeled, the more problematic the simulation will be and the more its results will deviate from physical reality.

1.4 The Future of Nanotechnology

The future of nanotechnology has been the subject of myriad books and articles, which span across many genres. Non-fiction books have included Drexler's *Engines of Creation*, John Storrs Hall's *Nanofuture: What's Next for Nanotechnology*,[13] *The Spike* by Damien Broderick,[14] Ray Kurzweil's *The Singularity Is Near*,[15] and investment books such as *Investing in Nanotechnology* by Jack Uldrich.[16] Fiction works include *Prey* by Michael Crichton[17] and Greg Bear's *Slant*.[18] These works cover nanotechnology in a wide variety of ways, from alarmism over technology run amok to Pollyanna-like predictions of a future utopia.

The discussion of the science and development of nanotechnology in this book emphasizes near-term issues and applications; our priority is more to characterize these properly than to offer speculative commentary which would very likely end up wrong. However, it is important to keep in mind the

[13] J. Storrs Hall, *Nanofuture: What's Next for Nanotechnology* (New York: Prometheus Books, 2005).
[14] Damien Broderick, *The Spike: How Our Lives Are Being Transformed by Rapidly Advancing Technologies* (New York: Forge Books, 2002).
[15] Ray Kurzweil, *The Singularity Is Near: When Humans Transcend Biology* (New York: Viking, 2005).
[16] Jack Uldrich, *Investing in Nanotechnology* (New York: Adams Media Corporation, 2006).
[17] Michael Crichton, *Prey* (New York: HarperCollins, 2002).
[18] Greg Bear, *Slant* (New York: Tor Books, 1998).