For many decades, nanotechnology has been developed with cooperation from researchers in several fields of studies including physics, chemistry, biology, material science, engineering, and computer science. In this paper, we explore the nanotechnology development community and identify the needs and opportunities of computer science research in nanotechnology. This paper is intended to benefit computer scientists who are keen to contribute their works to the field of nanotechnology and also nanotechnologists from other fields by making them aware of the opportunities from computer science. It is hoped that this may lead to the realization of our visions.

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1. Introduction

In 1959, Richard Feynman, a future Nobel Laureate, gave a visionary talk entitled “There’s Plenty of Room at the Bottom” on miniaturization to nanometre-scales. Later, the work of Drexler [1, 2] also gave futuristic visions of nanotechnology. Feynman and Drexler’s visions inspired many researchers in physics, material science, chemistry, biology and engineering to become nanotechnologists. Their visions were fundamental: since our ancestors made flint axes, we have been improving our technology to bring convenience into our everyday life. Today a computer can be carried with one hand – 40 years ago a computer (hundreds of times slower) was the size of a room. Miniaturization of microprocessors is currently in process at nanometre-scales [3]. Yet, the style of our modern technology is still the same as ancient technology that constructed a refined product from bulk materials. This style is referred to as bulk or top-down technology [1]. As conventional methods to miniaturise the size of transistors in silicon microprocessor chips will soon reach its limit and the modification of today’s top-down technology to produce nanoscale structures is difficult and expensive [3], a new generation of computer components will be required. Feynman and Drexler proposed a new style of technology, which assemble individual atoms or molecules into a refined product [1]. This Drexler terms molecular technology or bottom-up technology [1]. This bottom-up technology could be the answer for the computer industry. Though top-down technology currently remains the choice for constructing mass-produced devices, nanotechnologists are having increasing success in developing bottom-up technology [3].

There are some concerns regarding emergent bottom-up technology. First, the laws of physics do not always apply at nanometre-scales [4]. The properties of matter at nanometre-scales are governed by a complex combination of classical physics and quantum mechanics [4]. Nevertheless, bottom-up fabrication methods have been successfully used to make nanotubes and quantum dots [3]. These methods are not yet suitable for building complex electronic devices such as computer processors, not to mention nanoassemblies that can make copies of themselves and work together at a task. Furthermore, and significantly, once knowledge of nanotechnology is...
advanced and real-world nanoassemblers are realized, they must be properly controllable to prevent any threats to our world.

More recently computer science has become involved in nanotechnology. Such research is wide ranging and includes: software engineering, networking, internet security, image processing, virtual reality, human machine interface, artificial intelligence, and intelligent systems. Most work focuses on the development of research tools. For example, computer graphics and image processing have been used in nanomanipulators that provide researchers an interactive system interface to scanning-probe microscopes, which allow us to investigate and manipulate the surface at atomic scales [5, 6]. In addition, genetic algorithms have been used as a method in automatic system design for molecular nanotechnology [7].

Computer science offers more opportunities for nanotechnology. Soft Computing techniques such as swarm intelligence, genetic algorithms and cellular automata can enable systems with desirable emergent properties, for example growth, self-repair, and complex networks. Many researchers have successfully applied such techniques to real-world problems including complex control systems in manufacturing plants and air traffic control. With some modifications towards nanotechnology characteristics, these techniques can be applied to control a swarm of a trillion nanoassemblers or nanorobots (once realised). It is anticipated that soft computing methods such as these will overcome concerns about implications of nanotechnology, and prevent the notorious scenario of self-replicating nanorobots multiplying uncontrollably.

This article reviews nanotechnology from different points of view in different research areas. We discuss the development of the field at the present time, and examine some concerns regarding the field. We then focus on the needs and benefits of computer science for nanotechnology, as well as existing and future computer science research for nanotechnology.

2. Development in Nanotechnology

To describe Feynman’s grand visions that have inspired many researchers in several fields of study, Drexler introduced the term “Nanotechnology” and “Molecular Engineering” in his book, “Engines of Creation” [1]. He explored and characterized an extensive view of Feynman’s visions in many aspects including potential benefits and possible dangers to humanity. According to the vision, building products with atomic precision by bottom-up technology could offer a dramatic widespread of potential and a decrease in environmental impact which would improve our way of life. A simple example of potential benefits from nanotechnology is that information on papers could be packed into much smaller spaces so that less pollution from discarding those papers would be produced. The aspect that would be directly beneficial to humankind is nanomedicine, which involves medical research at nanoscale [1,8]. For example, a group of programmable nanorobots that could flow along our bloodstreams without harm to our bodies could be injected to treat our bodies from within.

Nanotechnology has indeed promised a great future for humanity. However, the down side of the technology should not be neglected. Drexler suggested the potential threats to life on Earth of uncontrollably replicating assemblers [1]. In order to prevent any threat to the society, it is crucial that nanotechnology is developed under acceptable standards with regard to ethical and social considerations. Recently, the Foresight Institute, which is a non-profit organisation for nanotechnology, gave version 4.0 of its guidelines as a self-assessment list for research and development in the field of nanotechnology [9]. The Science Media Centre has also produced a document describing nanotechnology for use by the media [10]. Today nanotechnology is gaining public attention. Many companies have been doing research and development in nanotechnology for commercial purposes. The governments of several countries have begun funding for research in this area. This recent development of nanotechnology is described further in the following sections.
2.1 Nanomanipulators

One important concept of nanotechnology is building products using bottom-up technology. Instead of sculpting bulk materials into desired products, bottom-up technology suggests a new method that assembles individual atoms into products. The first step to bottom-up technology is to acquire the ability to manipulate individual atoms at the scale of nanometres as desired. Therefore, the development of a nanomanipulator, which is a tool for manipulating nanoscopic materials, is seen by some as being crucial to the progress of nanotechnology.

The first imaging in nanoscale was from the electron microscope developed by M. Knoll and E. Ruska in 1931 [11]. Later in 1981, G. Binnig and H. Rohrer invented the scanning tunneling microscope (STM) that can image individual atoms, and earned the Nobel Prize [11]. The success of the scanning tunneling microscope leads to the development of other scanning probe microscopes (SPM) including the atomic force microscope (AFM). Instead of using lenses like traditional microscopes, all these scanning probe microscopes use a probe to scan atoms over the surface, measure a local property and result the image. Different types of scanning probe devices are designed for different tasks. For example, the STM is only appropriate when the material conducts electricity, while the AFM can work with non-conducting materials.

Apart from resembling a surface at atomic scale into a high-resolution image, scanning probe microscopes can be used to manipulate individual atoms. In 1990, D. M. Eigler of IBM used an STM to precisely place xenon atoms on a nickel plate into the name “IBM” [2, 12]. In 1993, W. Robinett and R. S. Williams developed a virtual reality system that allowed user to see and touch atoms via the scanning tunneling microscope [11, 13]. This was the beginning of a nanomanipulator. At the University of North Carolina, another nanomanipulator has been developed in a multi-disciplinary project involving in the collaboration of several departments including computer science, physics and chemistry. This nanomanipulator is a virtual-reality interface to scanning probe devices. Using technology in computer graphics, the features that are faint in the image can be enhanced. The system allows scientists to investigate and manipulate the surface of materials at the atomic scale. As a result, it has led to new discoveries in biology, material science and engineering. For example, scientists have used the nanomanipulator system to examine the mechanical and electrical properties of carbon nanotubes [6]. Nanomanipulators are now commercially available. However, the ability to manipulate individual atoms alone could not yet enable us to build reliable nanomachines, unless the physical principles at nanoscales are comprehended.

2.2 Nanofabrication

After scientists have gained the ability to manipulate individual atoms directly, the next step is to manufacture structures at nanometre scale, i.e. structures smaller than 100 nanometres across. In this section, we discuss nanofabrication methods, which can be divided into two categories: top-down methods and bottom-up methods [3, 14]. Akin to the concept of technology styles discussed previously, the top-down methods involve carving out or adding a small number of molecules to a surface, while the bottom-up methods assemble atoms or molecules into nanostructures.

A top-down method that has been used in the electronics industry is photolithography. Photolithography is the process that transfers the geometric shape on a mask to the surface of a silicon wafer by exposure to UV light through lenses. The computer industry uses this technology to fabricate microprocessor chips [3]. However, the use of photolithography to fabricate nanostructures is limited by the wavelength of the UV light. One modification can be made by using electron-beam lithography, which is a technique for creating fine patterns on a thin polymer film with a beam of electrons [3, 15]. Because electron-beam lithography is very expensive and slow, the development of soft lithography, which is a process that creates elastic stamp in order to transfer structures to a surface, allows researchers to reproduce patterns inexpensively in a wide range of materials. Nevertheless, this technique is not yet ideal for manufacturing complex multi-layered structure electronic devices. The need for methods to fabricate complex nanostructures that are simpler and less expensive has stimulated researchers to explore unconventional approaches.
Another top-down method involves using the scanning probe microscopes that were used to manipulate individual atoms to spell IBM. Researchers can manipulate atoms with an STM in three modes: pushing, pulling and sliding. Apart from mechanical manipulation, the STM can be used to assist in fabrication by chemistry catalyzing. In 1995, W. T. Muller et al proposed a method to use scanning probe microscopes in nanofabrication [16]. They used a platinum-coated AFM tip to scan over the surface coated with a monolayer of azide (-N3) compounds. As a result, amino groups are formed by catalytic conversions of azide and can be used to generate more complex structures. Another nanofabrication method using scanning probe devices was introduced by E. S. Snow and P. M. Campbell [17]. Their technique was to add a bias current to the AFM tip and monitor the electrical resistance of the structure during the fabrication process. When the target resistance is reached, the bias is switched off. This innovative feedback mechanism has been modified and used in later research. Recently, F. Rosei et al proposed a novel nanofabrication method for metal structures [18]. This method uses organic molecules as templates for the rearrangement of copper atoms on a surface. At low temperature where the copper atoms are static, the template molecules can be moved away without damaging the copper surface by precisely controlling the STM tip. For more information on using the scanning probe devices in fabrication, a review by S. W. Hla and K. H. Rieder is recommended [19].

In contrast, bottom-up methods are truly representing a new style of technology. Although the advancement of the bottom-up methods may not yet be suitable for the production of electronic devices or allow us to replace conventional top-up methods in fabrication, researchers can inexpensively assemble atoms and molecules into nanostructures with dimensions between 2 and 10 nanometres by self-assembly chemical reactions. One innovation created with a bottom-up method is a carbon nanotube discovered by S. Iijima of NEC in 1991 [11, 20]. A carbon nanotube is a tube-shaped carbon material that is measured in nanometre scales. It became the fifth type of solid-state carbon after diamond structures, graphite structures, non-crystalline structures and fullerene molecules or buckyballs, which were discovered by R. F. Curl et al in 1985 [11]. Since then, researchers have been studying the properties and characteristics of carbon nanotubes. Different structures of carbon nanotubes varying in length, thickness, type of spiral and number of layers have been developed for various purposes. Recently, NEC announced the world’s first compact fuel cell for mobile devices that uses spiral-shaped carbon nanotubes or nanohorns for the electrodes. Carbon nanotubes are expected to be a key material in the future.

Another new material, quantum dots, is made by bottom-up methods. Quantum dots are crystals that emit only one wavelength of light when their electrons are excited. Because the electrical, magnetic and optical properties of the dot are regulated by the size of the dot, the production of quantum dots must maintain their size and composition [3]. The size of the dots can be selected by varying the amount of time for the chemical reaction. The emission of light by quantum dots could be used in medicine as a biological marker [3]. Alternatively, quantum dots could be used as quantum bits and to form the basis of computers.

2.3 Nanocomputers

In 1965, G. Moore, the co-founder of Intel, predicted a trend that the number of transistors contained in a microprocessor chip would double approximately every 18 months. This became known as Moore’s law. As exemplified in Intel’s chips, the prediction appears surprisingly correct. However, with the development of nanotechnology researchers hope to break the barrier of Moore’s law.

One of the first achievements in nanocomputer research was perhaps the development of single-electron tunnelling (SET) transistors by D. Averin and K. Likharev in 1985/17. Later in 1987, T. A. Fulton and G. J. Dolan at Bell Laboratories fabricated single-electron transistors and made an observation on the quantum properties and effects of electrons when transistors are in operation [21]. As techniques in nanofabrication advances, researchers have successfully created electronic components including transistors, diodes, relays and logic gates from carbon nanotubes [22, 23]. The next step is providing the interconnection between components. Researchers have been working on a different type of nanoscale wires called semiconductor nanowires and studied how to interconnect and integrate the components [22]. The final step to build a computer...
processor is to fabricate the designed circuit. Recently, the semiconductor industry has successfully built 70-megabit memory chips containing over half billion transistors. As the advancement in nanofabrication progresses, the silicon-based nanocomputer will step closer into reality.

Another approach to nanocomputers is DNA computing. Deoxyribonucleic acid (DNA) is a nucleic acid that carries genetic information for the biological development of life. In 1994, L. Adleman introduced the idea of solving a well-known complex mathematical problem, called the travelling salesman problem, by using DNA [24]. His DNA computer showed that DNA could indeed be used to calculate complex mathematics; however, it is not yet comparable to conventional computer in terms of speed and ease of use. Nevertheless, his work has encouraged the development in DNA computing. In 1997, researchers at the University of Rochester built DNA logic gates, another step towards a DNA computer. The fact that a DNA molecule can store more information than any conventional memory chip and that DNA can be used to perform parallel computations make the area very appealing. Regardless of the success of DNA computers, the development of silicon-based nanocomputers could use the advantages of DNA computing.

Apart from silicon-based nanocomputers and DNA computers, researchers believe that quantum computers may be another promising approach that overcomes the limits of conventional computers [25]. Feynman began one of the first research groups to explore computational devices based on quantum mechanics. In 1982, he demonstrated how computations could be done by quantum systems according to the principles of quantum physics [26]. In quantum computers, the binary data in conventional computers are represented by quantum bits, or qubits, which can be in a state of 0, 1 and superposition (simultaneously both 0 and 1). As a quantum computer can hold multiple states simultaneously, it is argued that it has the potential to perform a million computations at the same time. However, quantum computers are based on quantum mechanical phenomena, which are vulnerable to the effects of noise. A scheme for quantum error correction is required. Researchers have been working to overcome this obstacle. To date, quantum computing is still in the very early stages.

2.4 Nanorobots

One vision of a nanoassembler or nanorobot is a device with robotic arms, motors, sensors and computer to control the behaviour, all at the scale of nanometres. In 1992, the book called “Nanosystem” by Drexler gives an analysis of the feasibility of machine components for such nanorobots [27]. However, even to build a molecular motor, researchers have to consider laws of thermodynamics when motors are actually in operation [28]. Just building a miniature version of an ordinary motor is not adequate. Recently, a controversy arose surrounding Feynman’s vision of nanorobots. In 2003, an open debate through letters between K. E. Drexler and R. E. Smalley (who was awarded a Nobel Prize for the discovery of fullerenes) was presented to public. Smalley was not convinced that such molecular assemblers envisioned by Drexler are physically possible, while Drexler insists on his previous findings. Certainly, the study of similarly-sized biological machines – organic cells – suggests there may be more effective alternatives to Drexler’s nanorobots. Even if nanorobots can be realised, they will not be available in the near future [29].

2.5 Nanomedicine

Nanotechnology promises a great future for medical research including improved medical sensors for diagnostics, augmentation of the immune system with medical nanomachines, rebuilding tissues, and tackling aging. Proponents claim that the application of nanotechnology to medicine, so-called nanomedicine, offers ultimate benefits for human life and society by eliminating all common diseases and all medical suffering [30]. Eventually, it is argued that nanomedicine would allow the extension of human capabilities. In 2003, R. A. Freitas Jr. commented that nanometre-scale structures and devices held great promises for the advancement of medicine including advanced biosensors, smart drugs and immunosolation therapies. In this initial stage of nanomedicine, nanostructured materials are being tested in various potential areas; for example, tagging nanoparticles using quantum dot nanocrystals as biological markers and
smart drugs that become active only in specific circumstances. In addition, researchers have found a method to control the size of densely packed DNA structures, one of nature’s efficient ways for transporting gene information. This could improve the efficiency of gene therapy for medical treatment and disease prevention. It is hoped by many that the next stage of nanomedicine, where nanorobots or nanocomputers are fully available, would expand enormously the effectiveness, comfort and speed of future medicine treatments with fewer risks and costs.

3. Benefits of Computer Science for Nanotechnology

Recently, M. C. Roco of the National Nanotechnology Initiative (NNI), an organisation officially founded in 2001 to initiate the coordination among agencies of nanometre-scale science and technology in the USA, gave a timeline for nanotechnology to reach commercialisation. For the next twenty years, the NNI has divided the development of nanotechnology into four generations. The first generation, which just ended in 2004, involved the development of passive nanostructures such as coatings, nanoparticles, nanostructured metals, polymers and ceramics. At the time of writing, we are at the end of second generation, during which we have manufacture active nanostructures including transistors, amplifiers, targeted drugs, actuators and adaptive structures [31, 32]. Later, from the year 2010, nanotechnology should enter the third generation. It is estimated that system of nanosystems, for example: guided molecular assembling systems, 3D networking and new system architectures for nanosystems, robotics and supramolecular devices, would be developed. Finally, from the year 2020, the fourth generation of nanotechnology should be the generation of molecular nanosystems, which would integrate evolutionary systems to design molecules as devices or components at atomic levels.

To date, nanotechnology has been developed mostly from the basis in physics, chemistry, material science and biology. As nanotechnology is a truly multi-disciplinary field, the cooperation between researchers in all related areas is crucial to the success of nanotechnology. Until now, computer science has taken a role mostly in research tools, for example: a virtual-reality system coupled to scanning probe devices in nanomanipulator project. However, according to M. C. Roco, the third and fourth generation of nanotechnology would rely heavily on research in computer science.

Perhaps reflecting the extensive use of computers in the modern world, computer science is today a broad field, with many aspects that may affect nanotechnology. Earlier sections have outlined the use of graphics and imaging with nanomanipulators. Other current uses of computer science for nanotechnology include developing software systems for design and simulation. A research group at NASA has been developing a software system, called NanoDesign, for investigating fullerene nanotechnology and designing molecular machines. The software architecture of NanoDesign is designed to support and enable their group to develop complex simulated molecular machines.

However, here we focus on intelligent systems. Research in intelligent systems involves the understanding and development of intelligent computing techniques as well as the application of these techniques for realworld tasks, often including problems in other research areas. The techniques in intelligent systems comprise methods or algorithms in artificial intelligence (AI) including knowledge representation/reasoning, machine learning and natural computing or soft computing.

An exciting new development at the time of writing is a project called PACE (programmable artificial cell evolution). This large interdisciplinary project aims to create a “nano-scale artificial protocell able to selfreplicate and evolve under controlled conditions”. The protocells in this work are intended to be the “simplest technically feasible elementary living units (artificial cells much simpler than current cells)”. These are intended to act as nanorobots, comprising an outer membrane, a metabolism, and peptide-DNA to encode information. Evolutionary modelling is being used extensively in PACE, to analyse real and simulated protocell dynamics, their possible evolution, and the evolution of (potentially noisy) protocellular networks. In addition to this work, computer modelling of embryogenesis and developmental systems is becoming increasingly popular in
computer science [33]. Should artificial cells become a reality, such models will provide a method for their genes to be programmed in order to enable the growth of larger, multicellular forms.

Apart from genetic algorithms and other evolutionary algorithms that have promising potential for a variety of problems (including automatic system design for molecular nanotechnology [7]), another emerging technique is swarm intelligence, which is inspired by the collective intelligence in social animals such as birds, ants, fish and termites. These social animals require no leader. Their collective behaviours emerge from interactions among individuals, in a process known as self-organisation. This collective intelligence in social animals often cannot emerge from direct interaction among individuals. Instead, indirect social interaction (stigmergy) must be employed. Each individual may not be intelligent, but together they perform complex collaborative behaviours. Typical uses of swarm intelligence are to assist the study of human social behaviour by observing other social animals and to solve various optimisation problems [34, 35]. There are three main types of swarm intelligence techniques: models of bird flocking, the ant colony optimisation (ACO) algorithm, and the particle swarm optimisation (PSO) algorithm. Different techniques are suitable for different problems.

Although still a young field of computer science, swarm intelligence is becoming established as a significant method for parallel processing and simultaneous control of many simple agents or particles in order to produce a desired emergent outcome. For example, researchers at the Santa Fe Institute developed a multi-agent software platform, called Swarm inspired by collaborative intelligence in social insects, for simulating complex adaptive systems. Likewise, BT’s Future Technologies Group developed a software platform known as EOS, for Evolutionary Algorithms (EAs) and ecosystem simulations. The group uses EOS for research into novel EAs and ecosystem models and for rapid development of telecommunication related applications [36]. Systems such as these will become increasingly important for modeling molecular machine systems. They are also being investigated as a solution to provide self-healing, adaptive and autonomous telecommunications networks. Another potential benefit of such techniques for complex adaptive systems in this area would be to control intelligently the manufacture of nanometre-scale devices, where no exact mathematical model of the system exists. Many intelligent systems’ techniques have been successfully applied in control system of various complex applications. Although at nanometrescale the principles and properties of materials are altered, researchers have attempted to solve other dynamic problems using soft computing techniques and have been developing new techniques to cope with such problems.

Also inspired by emergent collaborating behaviours of social insects, the Autonomous Nanotechnology Swarm (ANTS) architecture for space exploration by NASA Goddard Space Flight Center is claimed to be a revolutionary mission architecture. The ANTS architecture distributes autonomous units into swarms and organises them in hierarchy by using the concept of artificial intelligence. Researchers at the center have been developing a framework to realise the autonomous intelligent system by using an Evolvable Neural Interface (ENI). As a result, the interface allows cooperation between higher-level neural system (HLNS) for elementary purpose actions and lower-level neural system (LLNS) for problem solving as required in real-world situations. In the plan, each autonomous unit will be capable of adapting itself for its mission, and the ANTS structures will be based on carbon nanotube components.

In 1996, O. Holland and C. Melhuish investigated the abilities of single and multiple agents on a task with agents under similar circumstances as future nanorobots (minimal sensing, mobility, computation and environment) [37]. The task to be solved by the agents in their studies was to learn to move towards a light source by using simple rule-based algorithms. In the case of single agents, the result was efficient, but performance degraded as the amount of noise increased. In the case of multiple agents, the best result was from the algorithm that formed collective behaviours akin to genuine social insects. This investigation showed that emergent collective intelligence from social interactions among agents modelled on social insects could cope with the limited capabilities that would be inevitable in future nanoscale robots.

Recently, B. Kaewkamnerdpong and P. J. Bentley proposed a new swarm algorithm, called the Perceptive Particle Swarm Optimisation (PPSO) algorithm [38]. The PPSO algorithm is an extension of the conventional PSO algorithm for applications in the physical world. By taking into account both the social interaction among particles, and environmental interaction, the PPSO
algorithm simulates the emerging collective intelligence of social insects more closely than the conventional PSO algorithm; hence, the PPSO algorithm would be more appropriate for real-world physical control problems. This is the first particle swarm algorithm to be explicitly designed with nanotechnology in mind. Because each particle in the PPSO algorithm is highly simplified (each able to detect, influence or impact local neighbours in limited ways) and the algorithm is designed for working with a large number of particles, this algorithm would be truly suitable for programming or controlling the agents of nanotechnology (whether nanorobots, nanocomputers or DNA computers), whose abilities are limited, to perform effectively their tasks as envisioned.

This is seen as a crucial “missing link” in bottom-up nanotechnology: the control of the nano-sized agents. A billion (or trillion) tiny particles, whether complex molecules or miniature machines, must all cooperate and collaborate in order to produce the desired end result. None will have, individually, sufficient computing power to enable complex programming. Like the growth of crystals, the development of embryos, or the intelligent behaviour of ants, bottom-up nanotechnology must be achieved through collective, emergent behaviours, arising through simple interactions amongst itself and its environment. Computer science, and especially fields of research such as swarm intelligence, will be critical for the future of bottom-up nanotech.

4. Conclusion

As the development of nanotechnology progresses in several disciplines including physics, chemistry, biology and material science, computer scientists must be aware of their roles and brace themselves for the greater advancement of nanotechnology in the future. This paper has outlined the development of nanotechnology. It is hoped that this gentle review will benefit computer scientists who are keen to contribute their works to the field of nanotechnology. We also suggested the possible opportunities that computer science can offer, which can benefit other nanotechnologists from other fields by helping them be aware of the opportunities from computer science. This paper is intended to promote collaboration between computer scientists and other nanotechnologists.

As computer scientists who are interested in the field of nanotechnology, one of our future works is to build a system that consists of a large number of particles automatically forming into a designed structure. By using the PPSO algorithm to control the swarm of particles, each particle performs lightweight computations and holds only a few values. It is anticipated that models such as these will lead to successful bottom-up nanotechnology systems in the future.

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