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Nano-solutions for the 21st century

Unleashing the fourth technological revolution

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the 21st century

Acknowledgement

This work results from an extensive process that has included interaction and contributions by scientists, governments, philanthropists, and forward-thinkers around the world. Over the last three years workshops have been conducted in China, India, US, Europe, Japan, and more to discuss these findings and their global implications. Draft findings have also been presented at many meetings, from UNFCCC events to specialist conferences. The wealth of feedback received from this project has been of utmost importance and we see the resulting report as a collaboration project more than as the work of two individuals.

The authors wish to thank all those who have participated in the process and extend particular thanks to China and India, especially Institute for Urban & Environmental Studies, Chinese Academy of Social Sciences (CASS) and the team from the National Center for Nanoscience and Technology (NCNST) including Dr. ZHI Linjie, Dr. TANG Zhiyong, Dr. WEI Zhixiang and Dr. HAN Baohang. Professor Linjie Zhi was also kind enough to translate the abstract. In India the Rajiv Gandhi Foundation and CII - ITC Centre of Excellence for Sustainable Development were among those providing valuable input.

This report is only a start of what we hope is a vital international discussion about one of the most interesting fields of the 21st century. We would therefore like to extend special thanks to the Chinese Academy of Social Sciences (CASS), Chinese Academy of Sciences (CAS) and The Oxford Martin School which are examples of world leading institutions that support further discussions in this important area.

Dr. Eric Drexler and Dennis Pamlin worked together to make this report a reality. Drexler, currently at the Oxford Martin School, provided technical leadership and served as primary author of the report. Pamlin contributed through discussions, structure and input regarding overall trends in relation to the key aspects of the report. Both authors want to thank Dr. Stephanie Corchnoy who contributed to the research and editing. As always the sole responsibility for the content of report lies with the authors.

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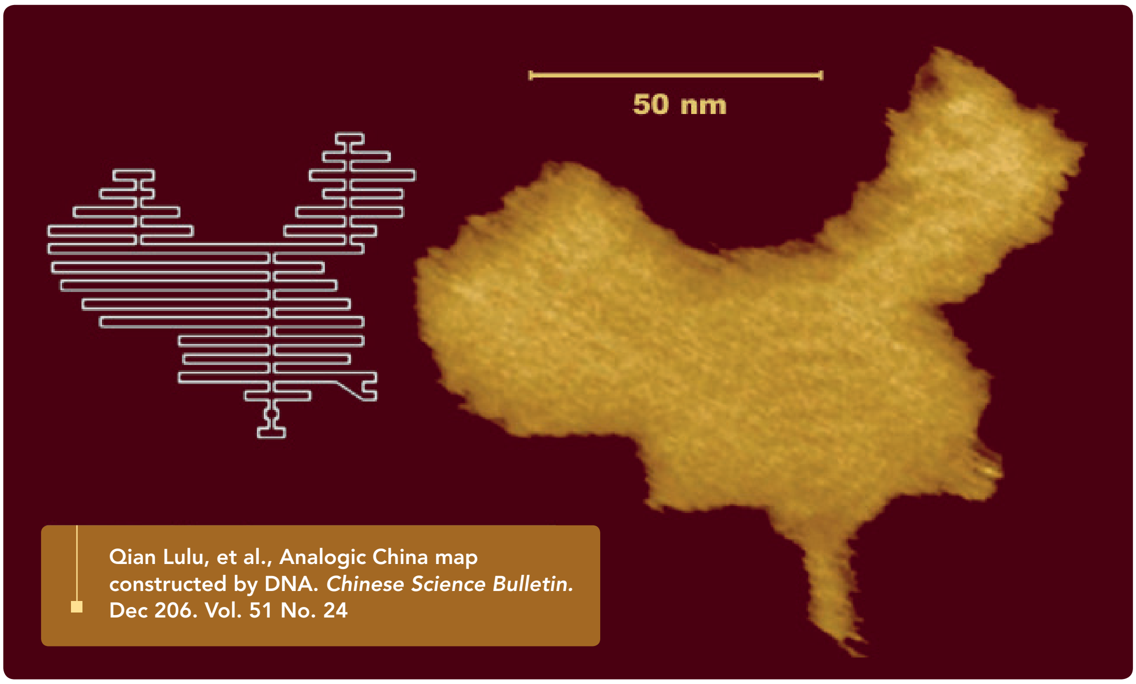

Qian Lulu, et al., Analogic China map constructed by DNA. *Chinese Science Bulletin.* Dec 206. Vol. 51 No. 24

Figure 1. An atomically precise biomolecular structure fabricated quickly and inexpensively by means of molecular self assembly. The structure contains approximately ½ million atoms. According to the taxonomy used in Table 4, this is a Level 2 nanotechnology.

Abstract:

The world faces unprecedented global challenges related to depleting natural resources, pollution, climate change, clean water, and poverty. These problems are directly linked to the physical characteristics of our current technology base for producing energy and material products. Deep and pervasive changes in this technology base can address these global problems at their most fundamental, physical level, by changing both the products and the means of production used by 21st century civilization. The key development is advanced, atomically precise manufacturing (APM).

This report examines the potential for nanotechnology to enable deeply transformative production technologies that can be developed through a series of advances that build on current nanotechnology research. The report has five sections:

1. *Nanotechnology and global challenge*
   The first section discusses the basics of advanced, atomically precise nanotechnology and explains how current and future solutions can help address global challenges. Key concepts are presented and different kinds of nanotechnology are discussed and compared.

2. *The birth of Nanotechnology*
   The second section discusses the development of nanotechnology, from the first vision fifty years ago, expanding via a scientific approach to atomically precise manufacturing thirty years ago, initial demonstrations of principle twenty years ago, to the last decade of accelerating success in developing key enabling technologies. The important role of emerging countries is discussed, with China as a leading example, together with an overview of the contrast between the promise and the results to date.

3. *Delivery of transformative nanotechnologies*
   Here the different aspects of APM that are needed to enable breakthrough advances in productive technologies are discussed. The necessary technology base can be developed through a series of coordinated advances along strategically chosen lines of research.

4. *Accelerating progress toward advanced nanotechnologies*
   This section discusses research initiatives that can enable and support advanced nanotechnology, on paths leading to APM, including integrated cross-disciplinary research and Identification of high-value applications and their requirements.

5. *Possible next steps*
   The final section provides a short summary of the opportunities and the possibilities to address institutional challenges of planning, resource allocation, evaluation, transparency, and collaboration as nanotechnology moves into its next phase of development: nanosystems engineering.

The report in its entirety provides a comprehensive overview of the current global condition, as well as notable opportunities and challenges. This content is divided into five independent sections that can be read and understood individually, allowing those with specific interests to access desired information more directly and easily. With all five sections taken together, the report as a whole describes low-cost actions that can help solve critical problems, create opportunities, reduce security risks, and help countries join and accelerate cooperative development of this global technological revolution. Of particular importance, several considerations are highlighted that strongly favor a policy of transparent, international, collaborative development.

Abstract:

当今世界正面临全球化的资源枯竭、环境污染、气候变暖、淡水缺乏、以及贫困等多方面的挑战。而这些问题的存在直接与我们当前的能源和材料的生产技术的特性密切相关。进入21世纪，广泛而深入的技术变革可以改变产品以及产品的生产方式，从而从根本上解决这些全球性问题。

这个报告分析了纳米技术在解决全球问题方面的潜力。根据目前的研究进展，纳米技术完全有可能通过一系列的发展进步成为具有深刻变革能力的生产技术。报告分为5个部分:

1. 纳米技术和全球性挑战
   第一部分介绍了纳米技术的基本内容以及纳米技术在现在和将来如何用于解决这些全球性的挑战。另外，有关纳米技术的主要概念和分类也在本部分做了介绍。
2. 纳米技术的诞生
   第二部分讨论了纳米技术的发展。从五十年前的第一次观察，到三十年前可以精确操纵原子，再到二十年前的一些重要研究成果，以及过去十年中一些重要单元的飞速发展。本部分以中国为例，讨论了新兴国家在纳米技术发展中的重要作用。
3. 变革的纳米技术
   这部分讨论了要使生产技术得到突破性进展所需的APM的不同的方面。通过战略性选择科研路线，以及多方面的协调发展，可以发展出生产必需的技术基础。
4. 加快发展先进纳米技术的步伐
   这部分讨论了研究创新可以实现并支持先进的纳米技术，如跨学科的综合研究和高价值的应用研究以及这些研究的需求。
5. 展望
   随着纳米技术向纳米系统工程阶段过渡，其在发展规划，资源分配，价值评估，透明度以及多方合作中面临着各种挑战。最后一部分简短地总结了纳米技术在这一阶段的发展过程中所面临的机遇以及解决这些问题的可能性。

报告的结构分成五个部分，这是为了让读者更容易找到他们感兴趣的部分阅读。整个报告旨在提供对当前形势、机遇和挑战的全面概述，每个部分都是独立的。作为一个整体，这份报告描述了一些低成本的途径，可以帮助解决关键问题，创造机会，降低风险，并且有助于不同国家加入并加快合作以发展这一全球性技术革命。一些观点有利于建立透明的国际化合作发展政策。

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PREFACE

More than 20 years ago I picked up Eric Drexler's book "Engines of Creation" and I was struck by its clarity and foresight.[1] It was not hard to understand that the ideas presented in the book would go through the same phases as most transformative ideas. First a period of hype when many are excited, then a revision phase where many try to redefine or dismiss the concept to make their current focus be seen as the most important. Then the issue disappears from the mainstream, even while people are developing and delivering the technologies that allow the transformative shift to happen. Then finally we reach the time for large scale implementation.

In the last 20 years, we have seen many new technologies go through these cycles, including the internet. For a younger generation it is probably unbelievable that only twenty years ago many dismissed internet and global connectivity as either impossible or a utopia. When the connectivity was a fact, things happened fast. Similar shifts have happened with the dematerialization of music, renewable energy (first wind and now solar PV), electric cars, and e-books. In each of these cases, people with technology understanding saw the potential, then hype discredited the ideas, and then came a "revolution" that was so "unexpected" that many companies and experts did not see it until it was over, and tried to cling to a world that was long gone.

Nanotechnology is now in a situation where the hype is over and the actual delivery has begun, but an important challenge in the case of nanotechnology, one that has created a lot of confusion, is that it is a "meta-tool". Nanotechnology is not a specific solution; it is more like fire, iron working, or semiconductor fabrication. When we talk about technologies today we often think about a final product like a car, computer, or camera. If we look a bit closer we might discuss things like an internal combustion engine, a CPU, a sensor. But we seldom look at what made these possible. In most cases, there is little news about this deeper level of technology. A closer look reveals that much of what we do today is based on incremental improvements over manufacturing technologies that are centuries old.

The advanced nanotechnology of High-Throughput Atomically Precise Manufacturing (HT-APM) will change all this, because it will open a new way to build and construct things. It will allow older ways of making things to yield to new, substantially better ways. This is not strange and has always been the case. For a long time iron working focused on things like making horse shoes, until this technology was used to make tools that led to new technologies that could make new things that we could use. So instead of just making horse shoes, the technology made it possible to make machines that could make cars.

Great progress has now been made toward the nanotech revolution as envisioned at the inception of the field in the late 1980s. This revolution leads to large-scale, low-cost, atomically precise manufacturing technologies with wide-ranging applications. The question is no longer whether there will be a revolution, but rather how transformative the revolution will be, and how fast it will happen. The pieces are coming together in different fields, and our decisions today will determine the speed and direction of transformative breakthroughs. These decisions will influence the outcome of the breakthroughs and how they affect global society.

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[1] Ten years later my discussions with Eric Drexler began. The first meeting took place more than a decade ago when I wrote an article for the Swedish government about the future of democracy. We met again when I was exploring the role of information technology and other converging trends in a project where I, together with Ewa Thorslund, wrote a report about a sustainable IT strategy. Then, during my time at WWF, we worked together to identify key applications of advanced nanotechnologies for sustainability. In my work as the Director for the Low Carbon Leaders, developed under the umbrella of the UN Global Compact project, different stakeholders interested in transformative solutions wanted to see a report about this kind of technology, as well as the policy framework needed to promote sustainable solutions. I'm grateful for the support I received for the earlier work as this report builds on this to a large degree.

High-Throughput Atomically Precise Manufacturing (HT-APM) will be the key threshold in advanced nanotechnology development, and it has the potential to be the most powerful tool humans have ever created. There is therefore a lot at stake. We are talking about deep changes in the material basis of global civilization that will take place in less than a generation, maybe even just a few decades, and these changes are of a magnitude comparable to all the technological advances that have occurred since the start of the industrial revolution.

When the magnitude of importance of the challenges we face is compared with the focus policymakers and business leaders have today, it becomes evident that we need a broad discussion of the way forward for research and development, and a discussion of scenarios that take account of these prospects.

When you are too close to something it is sometimes difficult to see it. When it comes to major changes in society, it can be difficult to see the rapid progress that is unfolding right in front of us. One reason is that the major changes are usually identified early by leading thinkers, but in media these ideas often turn into hype and unrealistic expectations of fast results. As research and development almost never live up to the short-term expectations that the most extreme proponents put forward and that make great headlines, the next step is a backlash where people don't talk about the transformative implications of longer-term progress, and talk instead about incremental improvements in existing systems.

People were talking about traveling without horses when the internal combustion engine was invented, but many did not see the change underway even when Ford was starting to pump cars out with the help of conveyor-belt assembly lines. Ford famously said that "if I'd asked customers what they wanted, they would have said 'a faster horse'".

Forty years ago people with knowledge about technology talked about a time in the future when use of paper and physical travel would be very different. Many people got excited, but business models that were built on selling printers/physical newspaper and travel agencies collaborating with airlines continued, and made change more difficult even though the technology existed. And now, while jokes about the paperless office continue, tablet computers and e-books are changing the ways we read media. In 2011 more e-books than "dead-tree books" are sold by the world's largest online retailer, and most people count the days until paper-based media no longer dominate the centuries-old business of book publishing.

In basic, physical terms, all the technological changes that we have experienced to date in human history are dwarfed in comparison with nanotechnology. The magnitude of change that nanotechnology will deliver, even in the most conservative scenario, is so extensive that most of our reference systems don't really help us.

Instead of brute force we now have the possibility to turn a page and work with nature instead of against it. High-Throughput Atomically Precise Manufacturing is a nanotechnology-based tool that is in front of us and as Dr. Eric Drexler writes we are the first generation that can simulate this future technology at a physical level, and use our knowledge to guide this upcoming industrial and technical revolution in the direction we want.

In a time of growing tensions, the potential to gather the world around a common challenge should not be ignored. So much of the focus today is on short-term gains (political and economic) that nanotechnology will be difficult to fit into existing structures, but this could also turn out to be a strength. New clusters could be established and new ways of collaboration could be developed. History is the only ultimate judge, but for anyone claiming global leadership in the 21st century, regardless of whether the focus is on poverty, environmental challenges, climate change, innovation or economic development, the prospects for transformative, nanotechnology-based developments must have a central role.

The increased collaboration regarding global challenges among the (re-)emerging countries could become a key vehicle to ensure that new solutions become part of the global agenda. Beside cooperation between the (re-)emerging countries we could also see global UN conferences and international standard development start integrating sustainable development of nanotechnology as a priority.

At the beginning of the 21st century, the key challenge is to create a fundamentally different approach in order to drive the necessary accelerated transition to a new economic model that can stop the climate crisis and create global well-being for nine to ten billion people.

We have to focus on how to meet the needs we have in a sustainable way rather than simply trying to eliminate problems in the current system. We have to look for integrated solutions that address climate change and poverty at the same time. The project will develop concrete proposals and strategies, based on key concepts that can deliver a sustainable low-carbon world without poverty. This report clearly demonstrates that nanotechnology should be one of the key priorities.

For 40 years, the dominating sustainable development approach has been problem-oriented. Now is the time to create a framework for transformative solutions, where cross-issue and cross-sector innovative collaboration approaches are used to create 21st century clusters that deliver 21st century solutions.

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NANOTECHNOLOGY AND GLOBAL CHALLENGES

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SIDEBAR 1

Trends, Challenges, and Nano-Solutions

Nanotechnology is climbing a ramp of capabilities that could address an increasing range of challenges. Below are examples of solutions that can help address three key trends. Of the following solutions, some are emerging products of current nanotechnology (E), others are anticipated products of more advanced nanotechnologies along paths leading to high-throughput atomically precise manufacturing (A).

Trend 1: Carbon emissions accelerating climate change

Solutions: Applications to energy production and efficiency{c8}

- Efficient solar electric power generation (E)
- Zero-net-carbon synthesis of fuels
- Efficient, high power-density fuel cells and batteries (E)
- Low-density, ultra-strong materials for vehicles (E)
- Thermal super-insulation for buildings (E)

Trend 2: Aging and health challenges

Solutions: Applications to medicine and public health

- Low-toxicity anti-cancer therapies
- Rapid production of curative treatments for emerging diseases
- Filters and chemical separation systems for purifying water
- Better-controlled production processes have no toxic emissions

Trend 3: Higher material welfare for increasing numbers of people

Solutions: Applications to processing materials and information

- Customized catalysts for transforming and synthesizing molecular structures
- Post-silicon computers and data storage
- High-throughput processing of molecules to make atomically precise nanoscale components (A)
- High-throughput assembly of nanoscale components to make macro-scale products

1. Nanotechnology and global challenges:

Understanding the material basis

1.1. Unprecedented global challenges require new solutions

The early 21st century is experiencing converging, global trends that bring both challenges and opportunities. The challenges are enormous: The limits of the planet are being encountered in areas ranging from the scarcity of natural resources to the inability to absorb increasing carbon emissions. At the same time, the number of people starving and living in poverty is growing in many places around the world.{c2}

These negative trends, however, are partly due to positive trends that include the elevation of increasing numbers of people to live in societies with high material welfare: food, medicine, transportation, and buildings that provide a comfortable environment. These positive trends are accelerating,{c3} yet they are thrusting the world toward a collision with physical limits.

SIDEBAR 2

Key terms and concepts used in this report [a]

It is important to distinguish between different kinds and levels of nanotechnology and how they relate to each other. The following provides an overview of some of the key concepts used in this report:

Productive nanosystems and atomic precision

A **nanosystem** is a device that functions by means of nanoscale components. A **productive nanosystem (PN)** is a nanosystem that can assemble small molecular building blocks under programmable control to produce **atomically precise (AP)** products (in other words, products in which every defect-free instance consists of an identical arrangement of atoms).

Biology and genetic engineering are based on productive nanosystems: Genetic information directs ribosomes to assemble chains of building blocks that fold to make atomically precise molecular structures and devices with diverse functions, such as powering motors, sensing pathogens, producing complex molecules, and converting sunlight into chemically stored energy. Anticipated artificial productive nanosystems span a range of technology levels that reaches from ribosome-like devices through factory-like systems of nanoscale machinery.

Atomically precise fabrication

Biological, chemical, and materials synthesis technologies can be used to perform **AP fabrication**. Their atomically precise products include pure organic molecules, biomolecules, nanoparticles, nanotubes, and nanomaterials of diverse kinds. Atomically precise fabrication is an enabling technology for developing artificial productive nanosystems.

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Mechanosynthesis

Productive nanosystems apply the principle of **mechanosynthesis**, a term that characterizes any process in which mechanically constrained motion brings reactive molecules together in controlled sequences and geometries. By restricting molecular encounters in this way, mechanosynthetic processes can control how molecules bond to form larger structures. This degree of control cannot be achieved in conventional processes in which reactive molecules diffuse freely and encounter each other at random.

Although the principle of mechanosynthesis has been demonstrated in both biological systems and laboratory experiments, the implementation of artificial productive nanosystems is only now becoming possible.

High-throughput atomically precise manufacturing

Atomically precise manufacturing (APM) refers to a class of anticipated production technologies based on artificial productive nanosystems.[b] These nanosystems may span a range of technology levels that begins with biomimetic, ribosome-like devices that assemble chains of building blocks, and later extends to include devices that assemble 2– and 3–dimensional structures composed of advanced materials of diverse kinds. These levels are characterized by differences in mechanosynthetic devices and the reactive molecules that they manipulate.

High-throughput **atomically precise manufacturing (HT-APM)** refers to a class of advanced APM systems with several characteristics: The use of coordinated, macroscale arrays of small productive nanosystems to implement atomically precise manufacturing of a wide range of macroscale products that exploit high-performance materials and devices. Fundamental mechanical scaling laws (see Background section B2) enable machines of this kind to operate with extraordinarily high throughput relative to current production technologies, as measured by mass processed per unit time per unit equipment mass.[c]

Lower-bound **HT-APM** refers to a class of reference systems selected to facilitate the derivation of high-confidence estimates of lower bounds on achievable system performance. The methodology for this is discussed in Section B5, and is based on consistent use of lower-bound estimates of performance for components and subsystems at all levels.

Nanotechnology

This report uses the term **'nanotechnology'** to refer to technologies that make or use structures in the nanometer size range, and the standard definition established by the U.S. National Nanotechnology Initiative extends this size range to 100 nm. These technologies can be directly useful in specialized applications; some of these are atomically precise, and some can serve as bridges to a series of progressively more advanced nanotechnologies that leads to HT-APM.

Outside the nanotechnology research community, the term **'nanotechnology'** is widely assumed to refer to technologies that involve atomically precise fabrication. This restrictive definition of the term contrasts with the broader and more recent size-based definition, which can, for example, designate irregular particles that contain tens of millions of atoms as products of nanotechnology.

It should be kept in mind that this clash in definitions led to conflicts during the political process that created the U.S. National Nanotechnology Initiative (2001) and determined the scope of the research that it would fund. During this conflict, leading advocates of the broad, size-based definition of the field popularized and criticized a false and impossible version of APM technology, and thereby generated widespread confusion regarding the content and scientific status of the actual, entirely different concept.

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Technology base

Every area of technology has a characteristic **technology base**, which is the set of tools, instruments, materials, components, and design methods that are used to implement the products of the technology. For example, the technology base for semiconductor manufacturing includes the wafers, photomasks, steppers, ultraviolet light sources, and so on, and the technology base for aerospace systems includes products of semiconductor manufacturing.

Level of technology

As used in this report, the **'level'** of a technology is characterized by the cost, performance, and range of different products that it can produce. The level of a technology advances with the level of its technology base.

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[a] These definitions follow the use of terminology in the Battelle/U.S. National Labs APM roadmap.

[b] The APM roadmap extends this definition to include the fabrication of atomically precise structures by means of scanning probe instruments.

[c] The term "high-throughput APM" is used in this report to provide a clearly distinguishing label for APM systems at a level of capability sufficient to transform methods of production across a wide range of industries.

Other long-term trends add complications. Both positive and negative trends take place at a time in history when societies are encountering increasing pressures for change as current institutions struggle with the consequences of rapid urbanization, an aging population, and an integrated economic system where fast financial flows can spread problems from one region to damage the global economy as a whole.

All of these trends are affected by another trend, one that has played a primary role historically both in solving and creating problems. This trend is the advancement of technology: the development of new products and production technologies. Today, technological development is faster than in any previous era, and in key areas, it is accelerating exponentially. The acceleration has multiple causes, including increased education and research funding, global collaboration, easier access to data, and the unprecedented combination and scientific understanding and computational simulation of the behavior of matter at a molecular level.{c5} Over the coming years we can expect key areas of technology development to continue their exponential rise, and nanotechnology is among them.

Nanotechnology can be seen from at least three perspectives. First, as a field that covers nanoscale and atomically precise developments in different existing fields, ranging from materials science to biomolecular engineering. Second, as a field that also covers the emerging fields where these and other existing fields meet each other and merge. Finally, as a field that is developing new atomically precise tools that can be used to make a next generation of better tools, in a cycle of technology improvement parallel to the rise of toolmaking from the earliest blacksmith's workshop to the modern automated factory—but this time, the cycle of technology improvement applies, not to hammered steel, but to organizing the fundamental building blocks of matter.

This line of development leads to extraordinary advances in products and production technologies, advances that would not be predicted by extrapolating trends. This is fortunate, because most extrapolations today lead deeper into a global crisis.

SIDEBAR 3

Understanding HT-APM: Principles and analogies

Simple analogies to conventional fabrication methods can suggest incorrect answers to fundamental questions regarding atomically precise manufacturing based on nanoscale factory systems. See also Background section B3, "The physical basis of atomically precise manufacturing".

Nanoscale semiconductor fabrication: The production equipment and processes have negligible similarities, and the products of semiconductor fabrication processes are not atomically precise. There is little basis for useful comparison.

Chemical synthesis: The processes and products are molecular, but reactive molecules move randomly, and limited control of how and where they combine severely limits the size and complexity of atomically precise products. Useful comparison is primarily at the level of individual molecular interactions.

Molecular biological processes: Atomically precise devices and processes guide critical molecular interactions, but their materials, structures, organization, and range of products are almost entirely unlike those of anticipated nanoscale factory systems. There can be little point-by-point comparison.

Conventional manufacturing: Enough mechanical and organizational principles of conventional factories apply at the nanoscale to make a point by point comparison useful, but at almost every point, the differences are large. For example, as discussed in Background section B2, at the nanoscale:

– Scaling laws increase machine operating frequencies by ~10^6.

– High operating frequencies increase throughput per mass by ~10^6.

– Moving parts rely on uniquely molecular phenomena for lubrication.

– Fixed parts are joined together by molecular interactions.

– Reactive molecules are brought together to direct molecular transformations.

– Thermal fluctuations and other nanoscale phenomena impose design constraints.

– From the nanoscale, assembly of components to make larger components spans tens of stages and a factor of ~10^9 in linear dimensions.

Digital information processing: In some respects, HT-APM resembles digital information processing. They share several characteristics:

– Devices are nanometers in scale and operate at high frequencies.

– Operations are applied to discrete entities (bits, atoms).

– Operations have discrete, correct or incorrect results (bits set, bonds formed).

– Thermal fluctuations (voltage, position) are potential error sources.

– Adequate tolerance margins in voltage and position can ensure low error rates $<< 10^{-9}$.

– Systems can be efficient and special-purpose or programmable and general-purpose.

– New systems can displace the products of multiple industries.

1.2. A unique moment in the history of science and technology

Our moment in history is unique in many ways, and one of them is this: Modern knowledge of physical law is sufficient to describe many of the properties of the fundamental building blocks of matter, atoms and molecules, and modern computational methods are—for structures of specific kinds, selected to be suitable for this purpose—sufficient to enable predictive dynamical modeling of atomically specified systems with sufficient accuracy to enable engineering calculations. For the first time in human history, it has become possible to gain a fundamental understanding of the capabilities of tools that cannot yet be built, thereby providing powerful insights into the achievable results of selected lines of technology development.

Table 1: The basis for expectations of low cost of HT-APM production. The physical nature of HT-APM enables estimates of incremental costs of production on a firm basis. The inputs are all of familiar kinds, with known costs. The cost of physical capital can be estimated because the production machinery is itself within the range of products. See discussion in Background section B3, "The physical basis of atomically precise manufacturing"

Cost source	Ratio	Basis for estimate
Materials	< 1/10	High-performance, low-mass products can be synthesized almost entirely from common materials such as CO_2, N_2, H_2O, Al_2O_3, and SiO_2.
Energy	~ 1	Mass reductions enabled by increased material performance are assumed to offset a moderately higher thermodynamic cost of material processing [1]
Labor	< 1/100	Molecular processing and successive assembly operations require no direct human intervention
Land	< 1/100	High throughput per unit mass and volume of manufacturing equipment enables a low footprint area
Machinery	< 1/100	High-throughput equipment can be manufactured by high-throughput equipment, diluting initial capital costs
Pollution	< 1/10	Reduced product mass requirements and precise control of processes and their by-products
Carbon emissions	~ 0	Production systems can be designed to operate with zero or negative net carbon emissions

[1] Backgrund section B3 notes thermodynamic limits and the requirement for several strongly exothermic process steps to implement reliable molecular-level operations in HT-APM.

Table 2. Four technological revolutions: Their technological basis for societal transformations of historic scale.

The Agricultural Revolution	
Provided new means of producing food and materials by exploiting the productive capabilities of the molecular nanosystems found in living organisms.	Encouraged stable settlement and land improvement, multiplied population densities by factors on the order of 10. Made possible the development of cities and civilization.
The Industrial Revolution	
Provided new means of producing material objects by exploiting the potential of artificial mechanical systems on a human scale.	Multiplied productive capacity by a net factor now on the order of 100, during a period of 200 years. Made possible new products, new ways of life, and ongoing changes in the structure of civilization.
The Information Revolution	
Provided new means of processing information using tiny, high-frequency components to manipulate and organize information in ultimate detail: patterns of bits in data.	Multiplied information processing capacity by an exponentially growing factor (roughly 2 per year), now $>10^9$. Made possible new kinds of information products and new ways to organize the material and human world, resulting in ongoing changes in the structure of society.
The APM Revolution	
Will provide new means of producing material objects: Like the Agricultural Revolution, it will exploit molecular nanosystems. Like the Industrial Revolution, it will use artificial mechanical systems. Like the Digital Revolution, it will use tiny, high-frequency components to manipulate and organize something in ultimate detail: patterns of atoms in products.	Compared to present industry, HT-APM will enable an enormous increase in throughput and efficiency of converting raw materials into high-performance, high-efficiency, zero-emission products, potentially multiplying productive capacity (measured by delivered product function, not mass) by a large factor (10 to 100) in a short time. Compared to present digital systems, the high performance of products of APM can increase machine capacities by $>10^9$. Compared to present agriculture, abundant but conventional capital stock can be used to optimize growing conditions. Experimental results which have demonstrated the potential to increase grain production per hectare by a factor of roughly 10. Can avert disastrous environmental effects of the Industrial Revolution, and willl make possible new products, new ways of life, and ongoing changes in the structure of civilization.

To do so requires careful design and analysis based on exploratory engineering methodologies and fundamental physical principles. For most scientists and engineers, this is a readily comprehensible kind of knowledge, yet the required methods of problem selection and analysis are not routine, and the results can be surprising. For the purpose of planning technology development this degree of insight into advanced objectives is potentially of great value. The methods are important to understand.

Early blacksmiths could not model automated factories, and could not conceive of these factories or conceive of a series of steps that would be sufficient to develop them. We, however, have far greater knowledge of science and engineering. This knowledge provides the ability to model a substantial range of atomically precise nanoscale machines and the ability to understand how a suitable set of machines could be organized to perform automated manufacturing (discussed in Background section B3). With this new and unfamiliar kind of knowledge, we have a basis for evaluating technology development objectives that are not currently within reach, and the ability to plan a program of science and technology development that will bring those objectives within reach (Chapter 4).

1.3. Global problems call for transformative change

The current global problems of resource supply, pollution, climate change, and economic development are directly linked to the physical characteristics of our current technology base for producing energy and material products. Deep and pervasive changes in this technology base can address these global problems at their most fundamental, physical level, by changing both the products and the means of production used by 21st century civilization.

The physical nature of this anticipated transformation of productive technology, high-throughput atomically precise manufacturing (HT-APM, Sidebar 3) can be understood through exploratory engineering based on understanding of the behavior of matter at a molecular level. The physical basis for developing this technology—advanced productive nanosystems—can emerge through a series of coordinated advances growing out of current research in nanotechnology.

It is difficult to assess the kinds of solutions that this fundamental transformation of productive technology can provide, but we can get a sense of scale by comparing it to the historical technological revolutions in which humanity first developed tools and methods for food production, then tools and methods for manufacturing material goods, now tools and methods to process information (Table 2). The Agricultural Revolution, the Industrial Revolution and the Information Revolution have all demonstrated how large-scale societal transformations are intimately linked to fundamental technological change.

The tools that advanced nanotechnology could provide will build on the earlier technological revolutions, but bring our capacity to shape and mimic nature to a new level. Atomically precise manufacturing can combine the molecular principles of biological production, the engineering principles of factory production, and the programmable flexibility made possible by the computing technologies of the information age. This is a powerful combination, offering a way to move beyond today's brute-force, fossil-fuel technologies and the problems they have created.

To meet today's challenges, incremental advances will not be enough. Success will require simultaneously expanding and replacing much of the world's physical infrastructure for power generation, transportation, housing, and manufacturing, and doing so at an economically unprecedented rate with technologies that in some instances do not yet exist in an economically viable form. A fully successful response to this challenge will require a pervasive and fundamental transformation of product and production technologies, a transformation that greatly improves product performance and greatly increases the rate at which new infrastructure can be deployed.

Ongoing progress in multiple fields of nanotechnology is enabling important, incremental improvements in product and production technologies, but this ongoing research progress is also building toward a technology base that can initiate developments of transformative scope. Using the challenges ahead as drivers for new solutions can accelerate research and development in the fields necessary to provide nanotechnologies that will meet crucial needs in the 21st century ranging from low-carbon solutions to new health applications.

1.4. Enormous change calls for systematic reevaluation of options and choices

The kind of capabilities that nanotechnology can provide over the coming years are so many and so significant that nanotechnology suffers from an unusual problem: It will provide so many solutions that are so transformative that it confuses people. It is important to distinguish clearly between technologies that are becoming available today and technologies that are objectives that will require a sustained development effort, and to distinguish both of these from speculations and fantasies about what might happen 100 years from now. To gain a firm grasp of the actual prospects, we need a framework for understanding what exists today, what is being developed today, and what scientific and engineering principles tell us can be developed in the future.

Applications of nanotechnology are already well advanced, with a growing impact on social and economic development in key fields ranging from materials and energy production to information technology and medicine. Ongoing innovations—new materials, new devices, new products—are widening the scope of nanotechnology. With anticipated advances in production technology, a far wider range of advanced products will become affordable, greatly widening their scale of application. These are aspects of an accelerating technological revolution that still has far to go.

We have entered a time of profound change, yet we must be careful to distinguish between sound scientific assessments and speculation. It is time to focus on the steps ahead and how to better integrate diverse technologies to build a technology base that can sustain higher and more productive levels of nanosystems engineering.

This report is meant to increase understanding of what solutions nanotechnology can provide, and in what time frame. It builds on the results of the Battelle/U.S. National Labs roadmap for atomically precise manufacturing[1] to explore existing research and how synergies can be created that can accelerate the development of a new generation of nanotechnology solutions.[12]

The report also suggests a framework to guide current research and development toward accelerated development of a new generation of nanotechnology solutions, with a focus on the development of a core technology base with a broad range of applications. Key elements of this framework are the establishment of criteria and metrics for evaluating research proposals and results with respect to their value as contributions to a coherent technology for nanosystems development, with a special focus on atomically precise nanosystems of special importance. In addition, it suggests criteria for institutional readiness and performance in a transparent, cooperative, and more efficient development process.

SIDEBAR 4

Nanotechnologies and environmental risks

Nanotechnologies can be a source of emissions that are toxic to people, or that have toxic ecosystem-level effects. In this area, it is important to distinguish between ordinary risks, and risks that are special to nanotechnologies.

Ordinary and special toxicity risks

The ordinary toxicity risks involve emissions of conventional toxic chemical substances into the air or water, either from industrial processes, or from the breakdown of products. As with any industry, these problems require monitoring and regulation, pushing industries toward green processes and non-toxic products.[21]

The special risks arise from biological exposure to nanoparticles, including nanoscale fibers and from their potential for unexpected toxic effects.[22] (It is important to recognize that nanoparticles are also common in nature and as by-products of combustion, and these also have distinctive toxicological properties.[23])

Nanoparticle-related toxicity is not always a concern, because many nanotechnologies make products with nanoscale features, not nanoparticles. Nanoelectronics and many nanomaterials technologies are in this conventional-risk category today, and many advanced nanosystems will be in this category in the future.

Why nanoparticles present special risks

Nanoscale particles and fibers are a major focus of nanotechnology research and development because they can produce enhanced or unique useful effects as a result of their size. For the same reason, however, they can also produce enhanced or unique toxic effects. They can enter the body, especially by inhalation, and some nanoparticles can enter the bloodstream and some of these can penetrate organs and cells throughout the body. Like chemical substances, some nanoparticles have toxic effects, and some bioaccumulate, while others are nontoxic or quickly metabolized or excreted, and these behaviors can depend on multiple physical and chemical conditions.[24] Similar remarks apply to transport, degradation, and effects in the environment.[25, 26]

What is special about regulating nanoparticles?

Much of what makes nanoparticles a special challenge is their diversity, complexity, and variability. Chemical substances consist of small particles, but these are atomically precise molecules, or well-defined mixtures. Nanoparticles contrast sharply with molecules in many respects: Typical nanoparticles are volumetrically billions of times larger than molecules, and in that volume, particles can vary across a continuous, many-dimensional continuum of chemical compositions. Particles of a single composition differ in size, internal structure, and surface composition and structure. Many of their properties depend on surface composition and structure, and these can change radically during aging or through exposure to different chemical environments.

In practical terms, what this means is that nanoparticles are difficult to characterize, define, and categorize. This, together with the novelty of their behavior, presents the main challenges to science and regulation, requiring both scientific study and institutional adaptation.[27]

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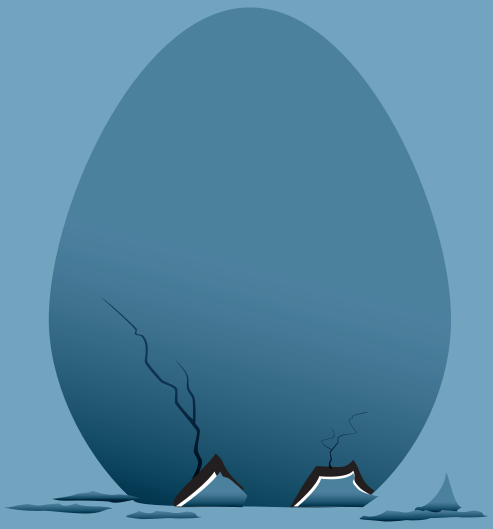

THE BIRTH OF NANOTECHNOLOGY

2

2. The Birth of Nanotechnology:

From Visionary Idea to World-Wide Research Delivering Initial Results in 50 years

Nanotechnology has been called a more significant industrial revolution than the internal combustion engine, and this view dates from the beginning of large-scale interest in this area of development. The judgment of policy makers regarding the importance of nanotechnology is indicated by the scale of world-wide support (as discussed below), and China, in particular, has given the field a high priority.

Support for nanotechnology research arises from two general sources: expectations for near-term results from incremental research, and expectations for revolutionary results from the eventual development of atomically precise manufacturing. The longer-term vision of atomically precise manufacturing came first (in the mid-1980s) and engendered the extraordinarily high expectations for nanotechnology; these expectations led to the emergence of public support for nanotechnology research in the 1990s. As a consequence of the resulting research progress, what had been a long-term vision in the 1980s has now become a technological objective within reach of a focused, multi-stage development effort.

The state of policy and opinion regarding nanotechnology and atomically precise manufacturing is the result of several influences:

- The extraordinary promise of atomically precise manufacturing, and the expectations that this raised.
- The ongoing achievements of the fields of research that have converged under the banner of 'nanotechnology'.
- The hype, misplaced expectations, and misinformation that have led to disillusionment regarding promises of revolutionary technological advances.
- The prospects for building on research achievements to develop atomically precise technologies that can fulfill promises of a broad and deep technological transformation.

2.1. The initial vision: A future revolution in atomically precise technology

In 1959, Nobel prize-winning physicist Richard Feynman proposed the fundamental concept of atomically precise fabrication: using nanoscale mechanical devices to build atomically precise structures by manipulating matter at the atomic level[13]. The basis for the modern concept of atomically precise manufacturing (APM), mechanically constrained motion of reactive molecules, was introduced in a 1981 scientific paper by an author of this report. This paper, together with a subsequent dissertation[15] and book-length analysis[16], described an approach to developing a technology that could manufacture atomically precise products with unprecedented capabilities, and that could do this at low cost (see Table 1). Further, the paper proposed a development path based on a biomolecular technology (protein engineering) that is now in an advanced state of development.

In 1986, the concept of atomically precise manufacturing was popularized under a name that was, at the time, not in active use: 'nanotechnology'[17]. The term quickly became synonymous with future technologies (sometimes realistic and sometimes fanciful or impossible) that were proposed to be potential products of atomically precise manufacturing. In the U.S., the excitement engendered by this vision of nanotechnology led to extensive newspaper and magazine coverage and caused the first surge of widespread interest in nanoscale technologies.

Table 3: Industries, AP technologies, and applications. Examples of industries and application areas in which Level-2 AP technologies promise substantial advantages. The physical basis for the advantages of nanoscale and AP technologies is discussed in Appendix.

AP fab capability	Industries	Production capability	Attractive products
Molecular fabrication	Chemicals	High-stability protein-like macro-molecules	Robust enzyme-like catalysts for fuel and chemical synthesis
Multi-component self-assembly	Manufacturing	Nanostructured multi-functional materials	Photovoltaics, fuel cells, medical implants, novel products
Networks of components	IT technology	Precise 3D configurations of active components	Displays, memory devices, computer chips, optoelectronics
Materials synthesis with control of form	Aerospace	Meter-scale, advanced-material structures	Ultra-strong, low-mass structures for aerospace vehicles

This led to growing public support for research in the area from the late 1980s to the 1990s, culminating in the year 2000 decision of President Clinton and the US Congress to fund a proposed Federal-level initiative in nanotechnology research. This decision was based on the promise that nanotechnology research would lead to a broadly applicable technology for atomically precise fabrication.[18]

In short, the vision of nanotechnology as a deeply transformative technology for atomically precise manufacturing shaped the field in several ways. Although the organized research community has adopted a definition of 'nanotechnology' that is based on feature size (and hence encompasses a far wider range of research areas),[19] the term is widely used to refer to technologies for making things with atomic precision.[20] In the U.S., this vision engendered not only the initial public excitement and the subsequent political support for funding a Federal initiative, but also the ongoing expectations of many members of the pubic and the political leadership. This has set the context for the development of concrete research programs.

2.2. The ongoing programs:
High-payoff research in nanoscale technology

Allthough usage varies, the standard technical definition of nanotechnology today now embraces a wide range of technologies, not necessarily atomically precise, that have features on a nanometer scale (1 to 100 nm).

Since the early 1990s, nanotechnology research has discovered a host of nanoscale structures, materials, phenomena, and devices that have technological potential that can be delivered relatively quickly. These technologies exploit a wide range of relatively specialized fabrication and materials processing technologies. Some of them use or contribute to the current set of atomically precise fabrication technologies, others do not.

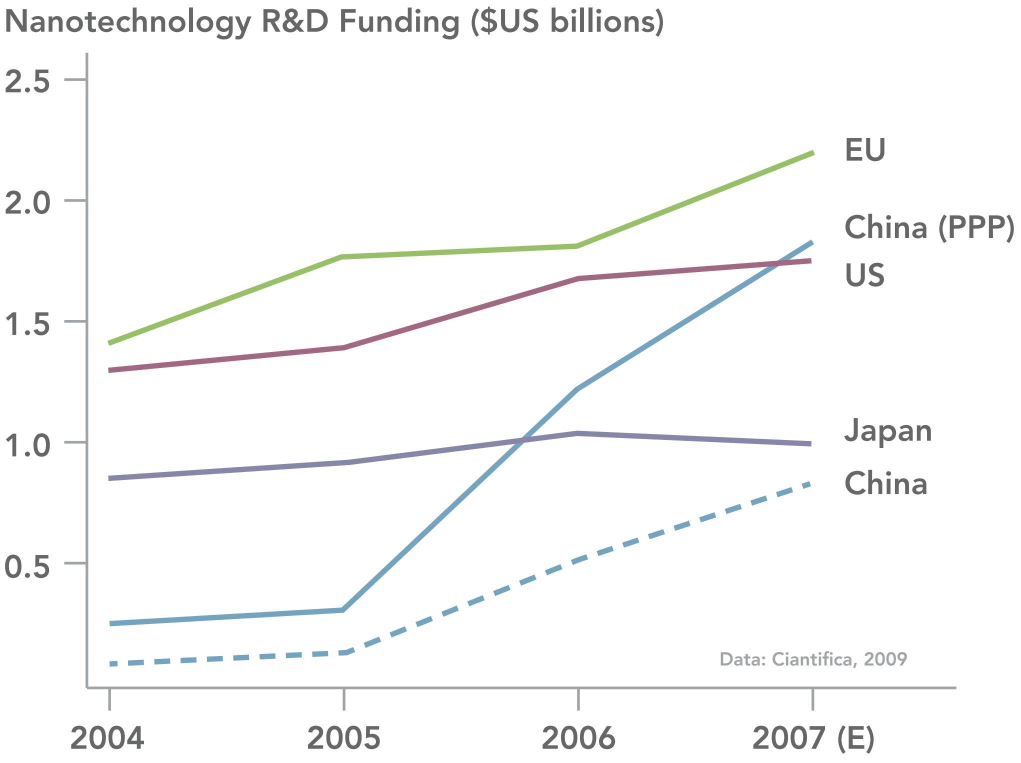

Figure 2. Growth and scale of nanotechnology R&D funding.[36]

To explore and exploit this closer-to-hand potential, diverse fields of science and technology have converged on research at the nanometer scale.

These fields and some of their nano-related areas of research include:

- **Materials science:** ceramics, metallurgy, polymer science, composites, nano-particles, -rods, -tubes
- **Chemical synthesis:** organic and inorganic synthesis, supramolecular chemistry, biomimetics
- **Semiconductor technology:** nanolithography, deposition and etching methods, device physics
- **Surface science:** surface characterization and modification, scanning probe atomic and molecular imaging and manipulation
- **Molecular bioscience and biotechnology:** biochemistry, molecular biology, biomolecular engineering
- **Biomedicine:** cell science, in-vivo imaging, biochemical analysis, immunological techniques, particle/cell interactions
- **Nanosystems fabrication:** production of multi-component systems using multiple materials and techniques
- **Computational modeling:** quantum chemistry, molecular dynamics, multiscale modeling, applied to of all of the above areas

Atomically precise fabrication methods have been developed in chemical synthesis, biomolecular engineering, and materials science. Many of the research areas listed above are either exploiting or extending these methods, and many are contributing to a technology base that enables further advances in atomically precise fabrication.

One early example of concrete progress was an experiment indicating that positional molecular assembly is possible. This experiment was performed by Ho and Lee at Cornell University in 1999. They used a scanning tunneling microscope to move an individual carbon monoxide molecule (CO) to an individual iron atom (Fe) sitting on a flat silver crystal, and chemically bound the CO to the Fe by applying a voltage

The application areas for actual and potential nanotechnology products are at least as diverse as the contributing fields of research. These application areas include:

- **Energy systems:** photovoltaics, batteries, fuel cells, fuel synthesis; carbon capture, energy conservation, power transmission
- **Transportation:** ground and aerospace vehicle structures (improved strength, lower weight); battery and fuel-cell propulsion systems
- **Information:** post-silicon device miniaturization, reducing power consumption, advanced display technologies
- **Medicine:** rapid response to emerging diseases; new therapies for cancers and viral diseases; diagnostic instrumentation; implants and artificial organs
- **Processing systems:** water purification, chemical purification, industrial catalysts, biomolecular and advanced materials synthesis
- **Manufacturing:** diverse areas of product improvement and innovation; reductions in cost, emissions, energy, and raw material consumption

The field of nanotechnology has brought together many other fields, and considered as a whole, it is part of an even broader convergence that includes biological, information, and cognitive technologies ("nano-info-bio-cogno").[28] These have been described as "becoming more and more the decisive factor of the race between regions and nations to win the future markets and society's wealth and political stability".

Near-term technological potential has been a primary motivation for the world-wide rise in nanotechnology research. A natural consequence of this research has been progress toward a technology base able to support the implementation of high-throughput atomically precise manufacturing. As discussed in Section {s 4}, progress in this direction can be substantially accelerated by identifying and supporting areas of research that serve objectives at both levels.

2.3. The mythical 'trillion-dollar nanotechnology market'

It is often said that estimates of what can be accomplished quickly are usually too high, while estimates of what can be accomplished through sustained effort are usually too low. Expectations regarding nanotechnology fit this pattern.

In 2001, a US National Science Foundation publication forecast a market of $1 trillion for nanotechnology-enabled products in 2015,[29] and subsequent estimates grew even larger. These market statistics, however, both exaggerate and underestimate the value of nanotechnology research.

Because of their basis, the usefulness of statistics and projections of "nanotechnology-enabled products" has been severely criticized.[30] For example, a 2007 report predicts a US$ 1.5 trillion "global nanotechnology market" in 2015, but the report then notes that "this is not the total value of nanotechnologies included in products, but the total value of the products. Thus a tenth of a gram of nanomaterials costing 10 cents may be included in a drug costing $100 per dose."

Using statistics based on the same principle, because the global automobile and construction industries use paint, they could be described as part of a multi-trillion-dollar "pigment-technology enabled" market. Statistics and projections of this sort are not useful as a basis for formulating research policy or economic plans.

The promise of high-throughput APM established extraordinarily high expectations for advanced nanotechnology, and inflated statistics have transferred some of those expectations to areas of research that cannot fulfill them. This has led some external observers to a degree of disappointment with progress in the field.

Nanotechnology market size does not measure economic or societal value

The trillion-dollar market-size estimate includes too much, yet it also includes too little. From a policy maker's perspective, decisions regarding investment in nanotechnology need to take into account considerations that are outside the scope of market size. They involve, first, societal return on investment, and second, the value of progress toward atomically precise manufacturing.

The first consideration is that the true societal value of new products can be far greater than the monetary value of sales or profits associated with them. For example, publicly funded nanotechnology research may lead to a new catalytic material that enables the development of high-efficiency, low-cost, low-emission fuel cells to power automobiles. This development might then reduce imports and increase exports on the scale of a significant fraction of GDP, while serving public goals of reducing resource consumption and environmental impact. In this example, a nanotechnology research product would produce enormous societal value, and this value would be increased—not decreased—by reductions in the production cost and sale price of the critical nanotechnology components. Thus, the size of the market for the nanotechnology product might be tiny, but the societal return on investment for the publicly funded research that created it would be very large.

The second consideration is that many areas of nanotechnology research are contributing to advances in atomically precise fabrication that could have a special longer-term value. This work can lead to incremental progress and direct applications, but it is advancing toward a technology base that will enable accelerating progress toward high-throughput APM. Through the achievement of HT-APM technologies, nanotechnology can fulfill its original promise and enable a technological revolution that is indeed quantitatively and qualitatively comparable to the Agricultural, Industrial, and Information Revolutions (Table {t 2}). The value of this has the potential to far exceed what has been promised by the trillion-dollar projections.

2.4. Nanotechnology research investment, a closer look at China

The world is increasing the investment in nano-related research. Unlike previous technology revolutions, nanotechnology research is more balanced and collaborative across the world. Emerging technology powers, like China, are playing an increasingly influential role. China has given nanotechnology research a high priority.[32] China's 10th and 11th five year plans emphasized objectives in nanotechnology, and nanotechnology is one of the four "science megaprojects"[33] in the State Council's 15-year National Long- and Medium-Term Plan for Science and Technology Development (2006–2020).[34]

International estimates of relative spending levels are difficult, but some observers believe that government investment in nanotechnology in China has surpassed that in the U.S. on a purchasing-power-parity basis (Figure 2). The numbers of Chinese nanotechnology patents and research papers have increased rapidly,[35] as have paper citation rates and the proportion of Chinese research papers in leading international journals.[36]

The magnitude of the research and development effort that is contributing to nanotechnology is larger than these estimates suggest. Methods of chemical synthesis are an essential part of the technology base for nanotechnologies,[37] yet most research in this area is not included as part of research in nanotechnology. Advances in quantum chemistry and molecular dynamics provide essential support for laboratory research, enabling the prediction and interpretation of physical behaviors. Commercial semiconductor lithography is often omitted, even though fabrication processes and products now operate deep in the nanoscale range and provide a potential basis for interfacing to atomically precise nanosystems.

The biomolecular sciences, including biomolecular engineering, are also often neglected as contributors to nanotechnology, yet biomolecular engineering of protein and DNA structures now produces the most intricate atomically precise structures that have been made to date.[38] The four "science megaprojects" in China's 15-year plan for science and technology development include "Nanotechnology" and "Protein Science" as separate categories;[33] it is important to recognize and develop their area of overlap.

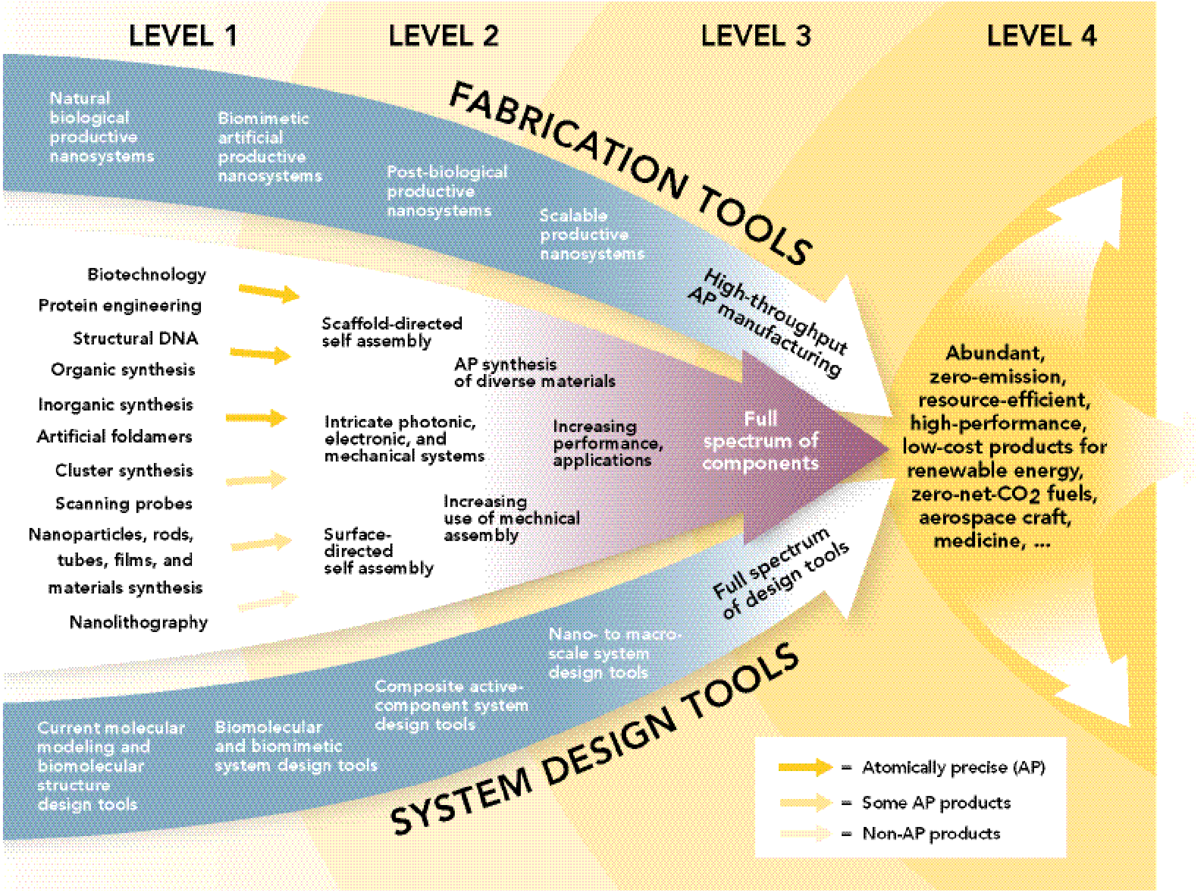

Figure 3. Converging technologies. Advances in multiple fields of nanotechnology are converging to enable the development of progressively more advanced nanosystems with increasing applications and global impact.

SIDEBAR 5

Areas of strength in Chinese nanotechnology research

A 2007 study of nanotechnology papers in the Science Citation Index{c76} identified 256 topical clusters, finding that "the US leads in 168, many times very heavily. China leads in 70 (many times very heavily). Japan leads in 15 (rarely heavily), and India, South Korea, and Spain each leads in one".

The study found China to be leading or dominant in 39 of the 58 topical clusters in the area of nanomaterials and nanoparticles, and "very dominant" in "synthesis of nanostructures". China also leads or dominates in several areas of nanotube research, and 19 of 35 topics in the area of polymers, composites, and metal complexes; these include areas of special significance to atomically precise nanotechnologies, such as structural characterization and synthesis of compounds (and of peptide compounds in particular), metal complexes and coordination polymers, and in X-ray and NMR methods for structural characterization.

The rank of Chinese nanotechnology publications, as measured by the ratio of highly cited papers to total papers was found to be very low in 1998, but at parity with Japan, Italy, and Spain by 2002.{76} Another study has found citation rates to Chinese papers to be increasing smoothly from 1994 through 2003, on a curve rising more steeply than the best exponential fit.{c77}

Research in nanotechnology and biomolecular technologies in China is expanding rapidly, and so this 2007 look at past publications can give only a rough idea of the current scope and scale of current research.

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DELIVERY OF TRANSFORMATIVE NANOTECHNOLOGY

3

3. Delivery of Transformative Nanotechnology:

Progress, Directions, Next Steps

Advances in multiple fields of molecular and nanoscale science and technology are converging to build a technology base that can enable systematic engineering of complex, atomically precise nanosystems. The next section discusses progress in the core enabling technologies, and the section that follows discusses the path ahead, outlining a series of increasing levels of atomically precise fabrication technology and their expected applications. These levels begin with incremental extensions of current AP fabrication technologies, followed by a series of advances in productive nanosystems technology, from technologies that exploit the programmable manufacturing machinery in biology, through biomimetic artificial PNs, and from there to increasingly factory-like systems on the path to high-throughput atomically precise manufacturing.

Incremental advances in the nanosystems technology base could lead to breakthrough capabilities in specific areas such as solar photovoltaics, batteries, fuel cells, nanoscale electronics, and medical therapeutics. As the level of fabrication technology approaches HT-APM, applications will expand rapidly, with far-reaching consequences.

3.1. Rapid progress in core enabling technologies

Researchers in nanotechnology have made progress in AP and AP-relevant fabrication in areas that include nanoparticles, chemistry, biotechnology, and materials science, among others. These diverse areas of research are building capabilities that, working together, can support the emerging technology of atomically precise nanosystems engineering. This supporting role for an emerging technology base must be considered when assessing the value of research in these areas, as it adds a component of value beyond that of immediate applications.

It is important to note that some of these areas are not themselves atomically precise (for example, nanolithography), but have characteristics that make them valuable in building systems that exploit the special properties of atomically precise components (Background section B2). Further, some of the areas make atomically precise structures, but are sometimes not considered to be examples of nanotechnology (for example, protein engineering).

The sections that follow outline some of the most important and prominent areas of research that are contributing to the development of AP nanosystems. The list is not comprehensive. Some high-payoff areas are listed here, yet would score highly if evaluated by appropriate criteria and metrics, such as (for example) atomic precision, structural stability, structural complexity, speed of synthesis, and range of functional properties. (Backgrund section B4 discusses the benefits of applying a criteria and metrics approach to evaluating research proposals and results.)

3.1.1. AP and non-AP technologies are complementary

Putting the pieces together

It is important to recognize that AP and non-AP nanotechnologies are in many ways complementary. AP components can potentially add value to non-AP system-building technologies (for example, as plug-in components for nanoscale semiconductor electronic systems, and non-AP components can potentially add value to AP systems-building technologies (for example, as active sensing elements organized and connected in a DNA framework). The experimental use of DNA linkers to enhance metal-nanoparticle sensors is one of many early examples.[39]

Combining AP and non–AP nanotechnologies

The structures made or studied in the technology areas highlighted above are atomically precise to varying degrees. Pure compounds of all kinds, including biomolecules, are fully atomically precise, while nanoparticles and other nanostructures range from fully atomically precise, to partially atomically precise to entirely irregular. Examples of the middle category include, for example, nanocrystals with areas of precisely structured surface, and nanotubes that are precise everywhere except at their ends. The common products of nanolithography have no reliable atomic regularity.

The range of non-AP functional components is immense, stretching from electronics and optics to catalysis and mechanical actuation. It is natural for applications to exploit these powerful non-AP technologies by employing synergistic combinations of AP and non-AP components. A system built using AP structural components as a framework for non-AP components would gain the benefits of precision and uniformity in the spatial organization of functional components of all kinds.

A device-level example: Single-molecule spectroscopy for sensors

For a device-level example, an AP framework could incorporate "sockets" that bind and orient non-AP metal nanorods. Similar devices have enabled optical detection and spectroscopy of single molecules[40], and the AP/non-AP self assembly approach could be used to make these plasmonic devices reproducibly in large numbers, while adding a range of capabilities by (for example) placing precisely-structured nanoscale molecular binding sites in the nanoscale sensitive region between rods.

A materials-level example: Semiconductor 'supracrystals' for optoelectronics

For a materials-level example, macromolecular AP structures that bind to non-AP semiconductor nanocrystals could be used to help control nanoparticle superlattice crystalization processes along the lines being explored in current research.[41] A very high degree of control and product complexity could be accomplished by encapsulating non-AP nanoparticles in AP macromolecular wrappers that would then undergo assembly directed by interactions between AP surfaces. Well-regimented nanocrystal superlattices would provide a way to implement miniband materials that have been proposed as a basis for solar photovoltaic cells of very high efficiency.[42] Regarding structures of this general class (organized ensembles of semiconductor nanocrystals), a recent review states that, with advances in fabrication technology, "The great diversity of such structures makes it possible to fabricate numerous ensemble-based devices for applications underlying photoluminescent devices, light-emitting diodes, displays, photodetectors, photovoltaic devices, and solar cells..."[43]

3.1.2. AP macromolecular engineering

- Protein and peptide engineering
- Structural DNA nanotechnology

By the metric of size and complexity, the leading AP fabrication technologies today are protein and DNA engineering, and these can play strongly complementary roles in an emerging technology based on framework-directed atomically precise self assembly. These and related molecules are the basis for AP structures and machines in biological systems, and they are manufactured in biological systems by digitally controlled productive nanosystems.

A 2006 breakthrough in structural DNA nanotechnology provides a fast and reliable method for designing and producing large, regular structures with hundreds to thousands of distinct, addressable 'sockets'. Protein nanostructures provide a way to bind other functional components (AP and non-AP, organic and inorganic) to specific sockets. The last 5 years have seen major advances in methods for design and fast production of these AP nanostructures. Together, these two AP self-assembly technologies provide a basis for developing a systematic methodology for fabricating complex, three-dimensional nanosystems with a wide range of components and applications.

3.1.3. AP products from chemical synthesis

- Complex molecules
- Modular molecular structures
- Crystal engineering

Chemical synthesis methods produce atomically precise components on scales typically ranging from a few to a few hundred atoms. Polymerization and crystalline self-assembly of these components can produce AP structures that reach larger and even macroscopic scales. Products of chemical synthesis serve roles that span all fields of nanotechnology.

Atomically precise design and fabrication originated in organic chemistry over 100 years ago, and means for producing complex AP molecular structures continue to multiply. In recent years, chemists have synthesized modular molecular structures that rival biomolecules in complexity and potential functional applications. Chemical synthesis also provides the building blocks used in the rapidly growing field of crystal engineering, and crystalline metal-organic frameworks can now be designed that form macroscopic, three-dimensional arrays of increasingly complex nanoscale structural units.

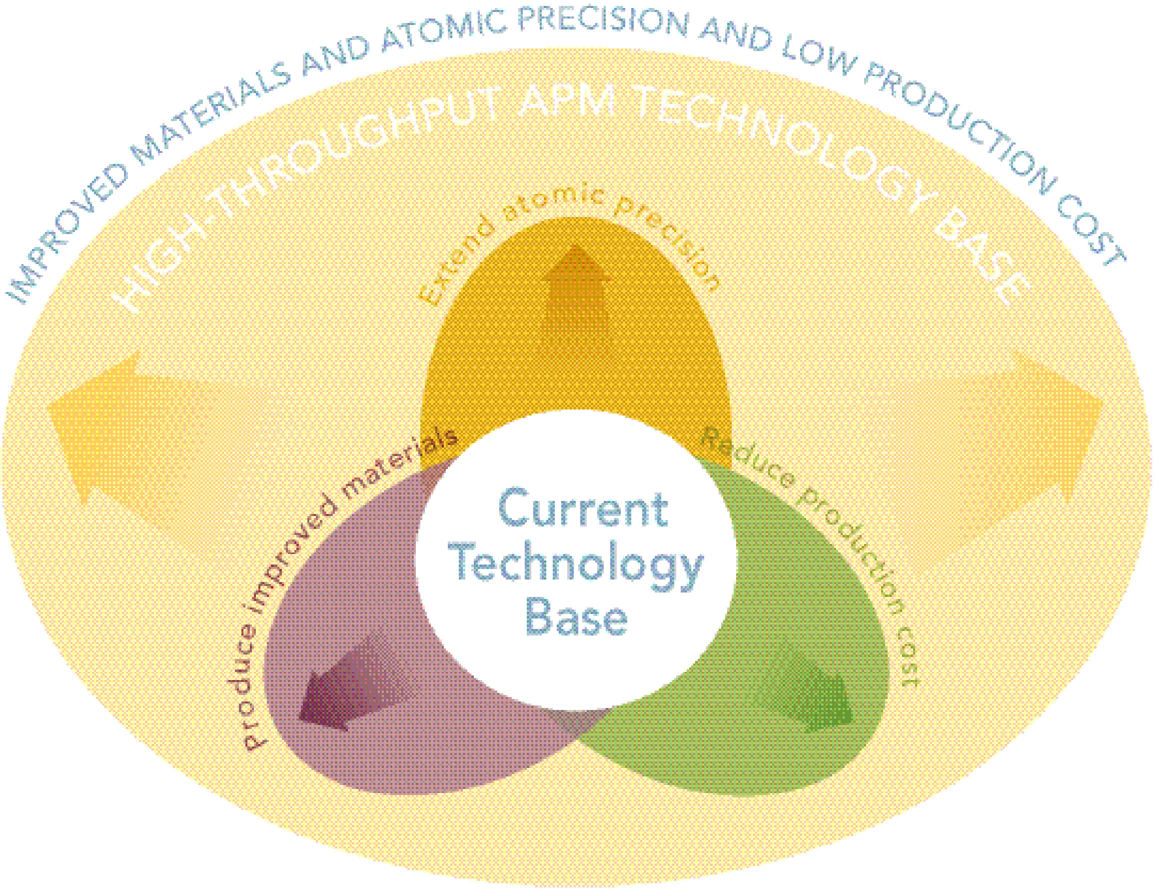


Figure 4. Expanding technological capabilities. Advances in nanotechnology are climbing a ladder of technologies that leads toward high-throughput atomically precise manufacturing (HT-APM). In combination, better materials, lower production cost, and atomically precise fabrication will expand technological capabilities synergistically.

3.1.4. General AP and non-AP nanostructures

- Nanoparticles, nanorods, nanotubes
- Systems made by nanolithography

Extraordinarily diverse methods are used to synthesize an extraordinarily diverse range of nanostructures with an extraordinary range of electronic, optical, mechanical, and chemical properties. China has played a large and growing role in developing these technologies.

Nanolithographic techniques are wide-ranging, their ongoing advance sustains the exponential, Moore's law advance of modern computing systems. In recent years, the scale of commercial nanolithographic structures has fallen below 30nm, creating a growing overlap with the size range of new framework-directed self assembled structures.

Some of these nanostructures are AP as a whole (e.g., closed-shell clusters) or in part (e.g., surfaces of nanocrystals, middle segments of nanotubes); others have no reliable atomic order (many nanoparticles, most nanolithographic structures). All, however, are candidates for integration with AP systems: small nanoscale structures can serve as components in systems organized by AP frameworks, and small AP systems can serve as components in systems organized by nanolithography. Recent work with organized DNA wrappings on carbon nanotubes illustrates one path toward interfacing small nanostructures with larger AP frameworks, and recent results from IBM illustrate one path toward interfacing large AP frameworks with even larger nanoelectronic systems, linking them to an enormous industrial technology base.

3.1.5. Computational modeling and design

- Computational quantum chemistry
- Computational molecular dynamics
- Computational macromolecular design

In macroscale systems engineering, computational modeling and simulation support computer aided design. For nanosystems engineering, the necessary modeling and simulation methods have advanced rapidly, enabled by advances in special-purpose software and general-purpose hardware. However, because the driving force behind these developments has been scientific needs in the molecular sciences, the development of nanosystems design tools that exploit this robust foundation has lagged. The emergence of macromolecular engineering methods is changing this situation.

Computational modeling of molecular phenomena originated in the 1950s.[44] It is only recently, however, that practical quantum chemistry (QC) methods (physics-based electron-level modeling) have been extended to describe bonding in molecules of significant size with chemical accuracy,[45] and only recently that molecular dynamics models (classical models based on empirical and QC-derived forces) have been extended to structure-size and time scales needed for describing macromolecular systems.[46] Meanwhile, simpler physical models combined with advanced design methods have recently enabled breakthrough advances in protein engineering (illustrated by the automated design of enzymes[47]), and even simpler design and modeling methods have supported the recent enormous growth in capabilities in structural DNA nanotechnology,[48] with landmark accomplishments in 3D structures published in 2009.[39]

SIDEBAR 6

Assessing contributions to the AP nanosystems technology base

In each of the current and emerging technology areas, there are particular lines of development of special importance to raising the nanosystems engineering technology base. For assessing fabrication processes and their products, favorable criteria and metrics include:

- Diversity of product materials and their properties
- Extent of atomic precision, especially on exposed surfaces
- Extent of controllable AP structural complexity
- Compatibility with aqueous processing
- Range of tolerance for thermal and chemical conditions
- Specific functional metrics for specific engineering roles

The development agenda for framework-directed self assembly

An area of growth today and great potential going forward is advancing the technology base for AP macromolecular self assembly. Because of their many applications in biotechnology, techniques for producing biological macromolecules are already powerful: The problem is not one of production, but of determining what to produce. This can be advanced by science, which can provide the information needed to improve predictive models, by computational design tools, which can enable engineers to explore and evaluate designs, and evolutionary methods, which enable the development of improved versions of a molecule by variation and selection using approaches that mimic biological evolution.

The research agenda for framework-directed self assembly highlights the importance of several areas. These include:

- Refining existing methods for engineering sequence-specific DNA-binding proteins; develop similar methods for non-biological synthetic foldamers (for example, peptoids, arylamides, and beta peptides).

- Developing more systematic methods for engineering protein-protein self assembly with control of geometry, including the integration of design and evolutionary methods

- Developing more effective methods for engineering specific binding of proteins to surfaces and nanocrystals with control of geometry

3.1.6. Atomic and near-atomic resolution imaging

- X-ray crystallography of proteins
- Scanning tunneling and atomic force microscopy
- Aberration-corrected transmission electron microscopy

In engineering design cycles, characterization of products is critical. Nanosystems engineering today centers on fabrication methods, placing structural characterization in a central role, and the most powerful methods are those that provide atomic and nearly atomic resolution structural data. Scanning probe microscopy achieved atomic resolution on surfaces in the 1980s, and has since then become a routine tool. Advances in transmission electron microscopy have recently enabled single-atom resolution of the interiors of robust, nanoscale inorganic structures. X-ray diffraction enables the determination of atomic resolution structures of molecules in crystals. This has been the single most powerful technique used to study the atomic-level structure of folded and self-assembled biomolecular structure. The scale of application has expanded to include ribosome structures[50] which are, of course, large and complex enough to implement programmable machines for atomically precise fabrication. Combinations of NMR spectroscopy and computational modeling can now yield atomically precise structures for proteins of substantial size.[51]

3.2. Raising the level of capabilities

Progress toward advanced nanotechnologies means progress in raising the technology base for designing and implementing nanosystems of progressively wider applications and progressively greater capabilities. There is no single, specific technology that is the key to progress. The process of raising a technology base (whether for chips or automobiles) requires advances in many different capabilities (different fabrication methods, materials, components) and there are usually many alternative ways to provide those capabilities.

There is, however, one kind of progress that is critical, because it ultimately sets the pace for the rest, and that is progress in fabrication technology.

No amount of scientific knowledge or clever design would have enabled a team of blacksmiths to make an automobile. Further, progress in making wheels and carts could make no direct contribution. To make an automobile required raising the technology base for fabrication: using tools to make better tools, step by step, ultimately building machine tools that could make better machine tools, and together with them, all the production equipment found in the automobile industry and its vast chains of suppliers.

The following three sections center on current, emerging, and anticipated levels of fabrication technology. The first focuses on the levels themselves, the second focuses on their applications to problem-solving technologies, and the third focuses on the steps that lead upward from present technologies through levels of fabrication technology that can provide progressively greater capabilities, maturing into the set of technologies that can enable high-throughput atomically precise manufacturing.

Recent developments in framework-directed self-assembly provide the basic elements of a long-anticipated technology[52] that can organize a wide range of biological and inorganic nanocomponents to form complex, three-dimensional nanosystems. In this approach to fabrication, an atomically precise molecular framework structure presents a defined spatial configuration of distinct, addressable “sockets”, each of which will strongly bind a specific, complementary “plug” attached to a specific type of functional component. Prototype implementations of this concept exist, and a wide range of fields can contribute to ongoing development. Examples of contributing areas include DNA scaffolds, protein adapters, and organic and inorganic components with diverse functions.

3.2.1. Building complex frameworks

Structural DNA nanotechnology provides the basis of current implementations of this concept. The distinct sockets are distinct DNA sequences, and the plugs (at present) are complementary DNA oligomers. Recent advances have enabled the construction of two- and three-dimensional DNA frameworks[53,49] that present hundreds of distinct binding sites in spatial configurations that can span hundreds of nanometers. Methods are becoming systematic and routine. Modified structures can be constructed in times measured in hours or days, hence the technology is compatible with a fast design-fabricate-test cycle for alternative configurations of components.

Table 4: A ladder of AP and AP-linked fabrication technologies. Each of the four levels of technology in the table enables the production of progressively more capable AP and hybrid nanosystems, including components and systems at the next level (see main text and PNTR[2]).

Technologies	*Fabrication capabilities*
Level 1: AP-linked core nanotechnologies	
Chemical synthesis	Greatest diversity of AP molecular products. Includes organic molecules, coordination polymers, and synthetic biopolymers. Many complex molecules are produced at >>10^3 tons/year.
Nanomaterials synthesis	Applies diverse techniques to diverse materials to make a wide range of nanoscale structures (particles, fibers, films, tubes...). Many of these have either fully or partially AP surfaces, and are scalable to >>10^3 tons/year.
Nanolithography	Produces complex nanosystems, including current digital electronics. Production scale >10^{11} units/year; active nanostructures ~100 tons/year. Non-AP structures, but now overlap the AP-structure length scale.
Biotechnology	Produces complex AP molecular products, both natural and engineered; these include industrial enzymes (production in China is approaching 10^6 tons/year)[78]
Level 2: Emerging AP methods	
AP macromolecular self assembly *(Based on nanoscale AP and AP-interface components)*	Intricate polymeric and composite macromolecular structures. Experimental production reaches >10^{12} structures of >10^6 atoms each. Components from chemical and biosynthesis and production potentially on a chemical/biotechnology scale. [1] Potential hybrid nanolithographic/self-assembled systems.
AP mechanical manipulation *(Based on macroscale scanning probe systems)*	Precise patterns of atoms on crystal surfaces. Typical experimental production: one structure of ~10^2 to ~10^3 atoms; throughput limited by number and speed of manipulating probes. Applications to science, molecular instrumentation, and prototyping of mechanical-PN processes.

(Table 4 continued)

Level 3: Artificial productive nanosystems	
Biomimetic PNs *(Based on sequenced binding and reactions of divalent monomers, comparable to ribosomes)*	Nanoscale AP structures and components based on high-performance polymeric materials. Applications as components of nanomaterials and self-assembled nanosystems. Cost per device <US$ 10^{-15} but the per-unit-mass cost of complex molecules used as feedstocks may be high (>1 US$/gm).
Machine-based PNs *(Based on spatial positioning and reactions of multivalent monomers or smaller reactive species)*	Nanoscale AP fabrication extended to ceramic, metal, semiconductor, and graphene. components. Increasing use of directed assembly at the systems level, and toward increasingly complex, high-performance products, common chemical feedstocks (~1 US$/kg), and larger-scale production [3]
Level 4: Scalable productive nanosystem arrays	
High-throughput APM *(Based on PN arrays and multistage component assembly)*	High-throughput atomically precise manufacturing of diverse products by means of arrays of machine-based PNs, followed by a series of stages of AP assembly that combine small components to make larger components (for example by convergent sequences that approximately double the linear scale of intermediate products at each stage).

[1] Developments in bacterial metabolic engineering have the potential to greatly reduce the cost of DNA[56]

[2] Ribosome-like fabrication of advanced polymeric components

[3] Precise, 3D control of growth of mixed oxide, semiconductor, metal, and covalent components for AP nanoelectronics and nanomachines; building blocks for larger structures

3.2.2. Expanding the range of components

To increase the scope of framework-directed self-assembly, it will be necessary to functionalize a wide range of components with ligands capable of sequence-specific DNA binding. DNA oligomers now serve this function, but their flexibility and dual role as framework components constrains their use. Zinc-finger proteins are attractive alternatives: They can be engineered to bind a specified base-pair sequence[54] and could provide a mechanically stiff attachment point for binding add-on components. Scaffold materials need not be functional components of fully assembled products, because they can be removed, or supplemented with other materials.

These products could consist, for example, of circuits made from inorganic nanoparticles and nanowires made of metals, oxides, and semiconductors, and in their final, functional form, they could reside directly on a nanolithographically patterned substrate.[55] Alternatively, the introduction of a high-stability organic or inorganic matrix material could lock components together while retaining a potentially very complex three dimensional organization.

SIDEBAR 7

Advances and directions in the molecular approach to atomically precise fabrication

The status of the key technologies

The technologies of biomolecular and chemical synthesis are now capable of fabricating a substantial range of complex, atomically precise structures. The most important of these are compact, polymeric structures (foldamers) and larger molecular scaffolds.

- Synthetic foldamers are now approaching the complexity of protein molecules, and can contain monomeric components with a wider range of functional properties.
- Protein engineering has recently reached the milestone of engineering new catalytic structures modeled on natural enzymes.
- Engineering molecular components that self-assemble to form new, complex crystalline materials has become routine.
- Structural DNA nanotechnology now enables the design and assembly of molecular scaffolds on a scale of millions of atoms and hundreds of nanometers.
- A rapidly developing design toolkit for self-assembly of diverse molecules and materials enables the construction of increasingly complex molecular systems.

Current research opportunities

These and related developments now make a range of experimental advances accessible. Some short-term goals and potential applications of the resulting technologies include the following:

- Demonstrate robust artificial foldamers that bind and stabilize complementary proteins.

– Enables development of enzymatic catalysts for use in relatively harsh industrial process conditions.

- Demonstrate enzyme-like foldamers that bind and determine the activity of synthetic transition metal catalysts.

– Enables development of highly stable and selective catalysts for the fine chemicals industry.

- Demonstrate self-assembled scaffolding structures that bind diverse components.

– Enables the organization of nanoscale electronic. optoelectronic, and plasmonic components to form nanoscale sensors and electronic circuits.

- Demonstrate self-assembled scaffolds that promote and direct the growth of inorganic nanocrystals.

– Enables production of atomically precise nanostructures with diverse materials and shapes for diverse applications in nanomaterials and nanosystems.

Middle-range objectives

Research opportunities today can open the door to the development of a next-generation technology platform that will, in turn, bring a new range of objectives into reach.

- The use of molecular scaffolds to bind and organize diverse components could be developed and elaborated to provide nanoelectronic fabrication methods for the post-Moore's-law era.

...continued

...continued

- Devices that link multiple catalytic centers (analogous to polyketide and polypeptide synthases) could be developed and elaborated to provide "molecular assembly lines" that convert small feedstock molecules into high-value macromolecular products in a single, integrated process.
- A capacity for directing the growth of nanocrystals and other non-polymeric structures could be developed and elaborated to provide a capacity for building entirely new classes of complex, high-performance, atomically precise nanoscale components and systems.

Accelerators

Progress toward these objectives can be accelerated by increasing the capacity for innovative design, and for reducing innovations to routine practice. The greatest needs today comprise:

- Design-oriented software that integrates levels of description and physical analysis that range from quantum chemistry through molecular mechanics to the continuum mechanics of materials.
- Design-oriented data repositories that describe available nanoscale and molecular components and fabrication methods.

3.2.3. Current challenges

As the technology of framework-directed self-assembly advances, multiple challenges must be overcome. For many applications, it will be necessary to reduce the frequency of structural defects in frameworks, or to discard defective structures. The thermodynamic properties of DNA hybridization are compatible with achieving very low defect rates, yet the frequency of AFM-observable defects in 100-nm scale frameworks is typically in the >10% range. [53] Impurities in starting materials, interfering reactions, kinetic traps, and damage caused by sample preparation and imaging are potential causes.

3.2.4. Wide-ranging applications

A system-building capability of this sort could potentially enable diverse applications such as multi-layer memory chips with petabit capacities, DNA sequencing chips able to read multiple human genomes per hour, and molecular tools and templates for next-generation atomically precise nanofabrication. Because DNA scaffold-directed self-assembly is in principle scalable to kilogram product quantities,[56] it holds promise for structuring materials on a scale suitable for applications in various 'smart materials', and in optoelectronic applications such as LED lighting, displays, and photovoltaics.[57]

3.3. Levels of nanotechnology: Fabrication

For convenience of discussion, existing and anticipated fabrication methods for nanosystems can be divided into four levels, and these four levels can be further divided into several specific technology areas. Each of the four levels of technology in Table 4 enables the production of progressively more capable AP (and partially AP) nanosystems, including components and systems of the kind needed to implement fabrication technologies at the next level.

In the table, the ***AP-linked core nanotechnologies*** are fabrication technologies in wide use today, that either make atomically precise products, or that make products that have natural utility in nanosystems with major AP components. Each of these fabrication technologies is the basis for a large or substantial industry.

The next level, ***Emerging AP methods***, contains fabrication methods that are available today, but are at an early phase of development.

The first area in level 2, ***AP macromolecular self assembly***, is strongly biomimetic: This is how biological systems build molecular machines, including biology's productive nanosystems. Structural DNA nanotechnology is based on macromolecular self assembly, protein engineering often relies on it, and non-biological foldamers have similar potential but based on a wider range of molecular structures and chemical properties. AP macromolecular self assembly is the basis for ongoing developments in framework-directed self assembly. Products can potentially be produced in bulk, aided by synthetic biology techniques.[57]

The second area, ***AP mechanical manipulation***, extends the use of directly controlled tools to the molecular and atomic scale. As first demonstrated in 1990,[58] scanning probe tools (AFM and STM) can be used to arrange atoms and molecules on surfaces with discrete, digital-precision control. This has been demonstrated in a diverse, growing, but still very restricted set of surfaces and operations. Limitations on throughput preclude scale-up to macroscopic production levels, but applications to high-value atomically-precise devices (e.g., sensors) are under investigation. This technology also has potential applications in prototyping operations to be performed by future high-throughput machine-based PNs.

In the groups that follow, the implementation of ***Biomimetic PNs*** is within reach of emerging AP macromolecular self-assembly techniques, but the implementation of ***Machine-based PNs*** will require components and assembly methods of greater capacity, and the implementation of ***Scalable productive nanosystem arrays*** will require an extension of machine-based PN technology, and provides the basis for ***High-throughput APM***. These technologies are understood based on physical and engineering principles (Background section B3).

3.4. Levels of nanotechnology: Applications

Increasing levels of fabrication capability enable applications of increasing capability, as measured by both the range of products and by their cost and performance metrics. Table {t 5} summarizes some of the major applications that can be expected as fabrication technologies advance.

The level of fabrication technology that will be required for a particular application to become feasible and practical is a matter for speculation, because experience shows that unexpected ways to solve problems can accelerate applications, while unexpected problems can delay them. The table reflects this uncertainty by attempting only a coarse categorization of applications, listing them in columns that correspond, respectively, to the first and second levels in Table 4 (core and emerging nanotechnologies), and to the third and fourth level (small, then scalable productive nanosystems).

Advanced applications can be more predictable

In comparing the products of more-advanced and less-advanced fabrication technologies, the capabilities of products of more-advanced technologies (or more accurately, *lower bounds* on those capabilities) can often be assessed with greater confidence than those of the products of less-advanced technologies. This may be surprising, because the products of the less advanced (current and emerging) technologies are closer, in the sense that they can be developed sooner.

Implementation and understanding, however, often do not correspond. Fabrication processes can work when they are not understood (for example, all chemical processes before the discovery of molecules), and can sometimes be understood when they cannot be implemented (for example, chemical processes directed by mechanical constraints on reactant positions). In the present case, the inverse relationship between degree of understanding and ease of implementation is a direct consequence of the greater control enabled by the more advanced processes, because greater control tends to lead to greater predictability. (Failing to recognize this inverse relationship can be a conceptual barrier to understanding HT-APM.)

In brief, higher-level fabrication technologies are more direct and systematic, and therefore some of their applications, although more advanced for these reasons, are for the same reasons more predictable than those of earlier levels.

There are several specific considerations that engender this differential in understanding.

Materials that are more stable and fine grained: A primary consideration is that the components produced by the progressively higher-level fabrication technologies can be progressively more stable and fine-grained, being constructed from small multivalent monomers or from smaller reactive chemical species. The products can be strongly bonded solids on a spectrum that extends from highly cross-linked polymers to oxides, metals, and covalent solids.

The properties of these materials contrast with those of currently accessible products of productive nanosystems, which are linear polymers with few or no cross links, relatively large monomers, and structures that depend on relatively weak, non-covalent binding forces to give them form and stability. (Note, however, that protein nanostructures can have mechanical properties like those of epoxies, polycarbonates, acrylics, and other engineering polymers.)

Better and more diverse functional components: A second consideration is that the ability to fabricate a wider range of AP product materials and structures will enable the fabrication of a wider range of functional components (mechanical, optical, electronic, and so forth). These can include components of kinds that are known today only from computational experiments, or from small-scale laboratory demonstrations of the physical properties of single nanostructures.

With current fabrication technologies, by contrast, control of molecular-level structure is highly indirect, and usually depends on manipulation of general variables such as temperature, solvents, and dissolved reactants. Experience shows that this control is often insufficient to produce predictable results, and can seldom produce uniform results (that is, AP structures) beyond the scale of macromolecules and extremely small nanocrystals.

More direct control of product assembly: A second consideration is the potential for greater and more direct control of product assembly. In the lower range of the technologies contributing to applications in the second column of Table {t 5}, self assembly is the natural means for joining components, and the use of more stable components, made with finer-grained control of surface structures, will facilitate the design of the required, unique and complementary interfaces, and can also increase the robustness of the interfaces formed when these complementary surfaces bind to each other. At more advanced levels, self assembly can be guided, and ultimately replaced, by mechanically constrained motions that bring components together and join them without relying on uniquely complementary surfaces. When extended, this approach leads to factory-style modes of organization, and hence to production systems that are highly predictable and controllable.

In combination, these three considerations imply that advanced fabrication technologies can enable greater ease of design and analysis for a wider range of products, and that they can enable greater confidence that known phenomena can be reproduced with reliability and implemented on a large scale. For systems and applications within this range of products, there is little question of their feasibility; the main questions involve the potential for fabricating them with earlier, less well understood technologies, and whether systems of a different kind will enable higher performance products than those that can be expected based on current knowledge. The latter uncertainty is the reason why this mode of analysis can provide only lower bounds on expected capabilities.

Table 5: Nanotechnology applications at earlier and more advanced levels of fabrication capability. The first column and second column in this table correspond to the first two groups and the second two groups of fabrication technologies in Table {t 4}. For reasons discussed in the text, the characteristics of applications in the second column are generally more predictable than those of applications in the first column.

Potential applications of core and emerging AP nanotechnologies	*Relatively predictable applications of microscale and meter-scale productive nanosystems*
Energy	
Improved gas separation membranes for carbon sequestration processes in coal-fired plants Quantum dots and quantum wires for high efficiency solar photovoltaics Nanostructured materials for improved fuel cells, batteries, and ultracapacitors More efficient catalysts and electrocatalysts for storing energy from renewable but intermittent sources (i.e., solar photovoltaics) in high-energy density fuels	Low-cost fabrication of complete energy production systems that include high-efficiency[1] solar photovoltaic arrays, energy storage systems, and power distribution systems Low-cost fabrication of high-power-density[2] packages that convert fuel and oxygen to shaft power, water, and stored CO2 Low-cost fabrication of high-power-density[2] devices that convert electrical energy, water, and CO$_2$ to fuels and oxygen
Mobility	
Lightweight, higher-strength composites to reduce vehicle mass Zero-net-emission power sources based on improved fuel cells, batteries, and ultracapacitors. Fuels from renewable energy sources.	Low-cost fabrication of complete vehicle systems from ultra-high performance materials and ultra-high performance, zero-emission power systems
Information	
Contributions to advanced nanolithography Development of post-silicon technologies for computational and information storage devices	Extremely low-power computational devices CPU sizes in the cubic-micron range Compact, low-power 109 CPU/machine systems

Medicine	
Accurate targeting of drug delivery to cancer cells Fast, low-cost genome sequencing during a patient’s office visit.	Complete molecular characterization of cells and tissues as a routine basis for medical research and diagnosis A broad range of applications made possible by micron-scale biocompatible devices with both molecular sensors and tools that perform actions under specified conditions and with algorithmic control
Processing and manufacturing	
Improved catalysts for more efficient, greener chemical processes Improved membranes for purification of water and chemical products Replacement of resource-intensive materials with nanostructured organic and silicate materials	Low-cost, resource conserving, moderate energy, zero-emission processes for the manufacture of materials and products of all of the kinds listed above, enabling large-scale production, widespread application, and transformative results for global problems of resource depletion, energy production, and emissions of CO_2 and of toxic waste products.
	[1] Efficiency >50% [2] Power density >1 kW/cm^3

3.5. Accelerating progress on the road to HT-APM

Iterative improvement in the PN technology base

Together with a suitable technology to support the design aspect of nanosystems engineering, early-generation productive nanosystems could be used to produce the components for improved, next-generation productive nanosystems. Directions for improvement of next-generation PNs include the ability to bind and position an expanded range of monomeric building blocks, and the ability to assemble them in more complex patterns. These extended capabilities enable the fabrication of improved materials and components, and with these, the production of a wider range of higher-performance products. Among the potential products are higher-performance PNs.

This process of iterative improvement, using PNs to build improved PNs, can potentially be used to climb a ladder of incremental improvements that leads through biomimetic PNs to machine-based PNs that are progressively larger and more capable. Biological productive nanosystems offer an attractive starting point.

Lines of advance toward advanced APM

There are lines of advance that lead from current capabilities to advanced APM. A range of potential approaches would fit this outline:

- Biological PNs and other tools and materials from AP-linked core nanotechnologies can enable the development of a broad technology base for engineering self-assembled AP macromolecular nanosystems with a wide range of functions.
- Self-assembly of biological PNs, which are AP macromolecular nanosystems, can serve as a general model for developing biomimetic artificial PNs. These can expand the technology base by enabling the production of macromolecules with new characteristics.
- New characteristics can include improved functional features, increased stability, and finer-grained control of structural design, thereby enabling more systematic design of complex, high-performance AP products. These products can include next-generation PNs that enable further advances.
- A natural line of PN development is to increase the use of mechanically guided motion to create complex assemblies in a direct and reliable way. This can incrementally displace self-assembly, thereby reducing design constraints, simplifying components, and enabling improved product performance.
- Higher performance components and direct, reliable assembly methods open the way to incremental development of systems in which arrays of PNs produce nanoscale components, and subsequent multi-stage assembly processes combine them to form macroscale products.

Improved technologies tend to accelerate improvement

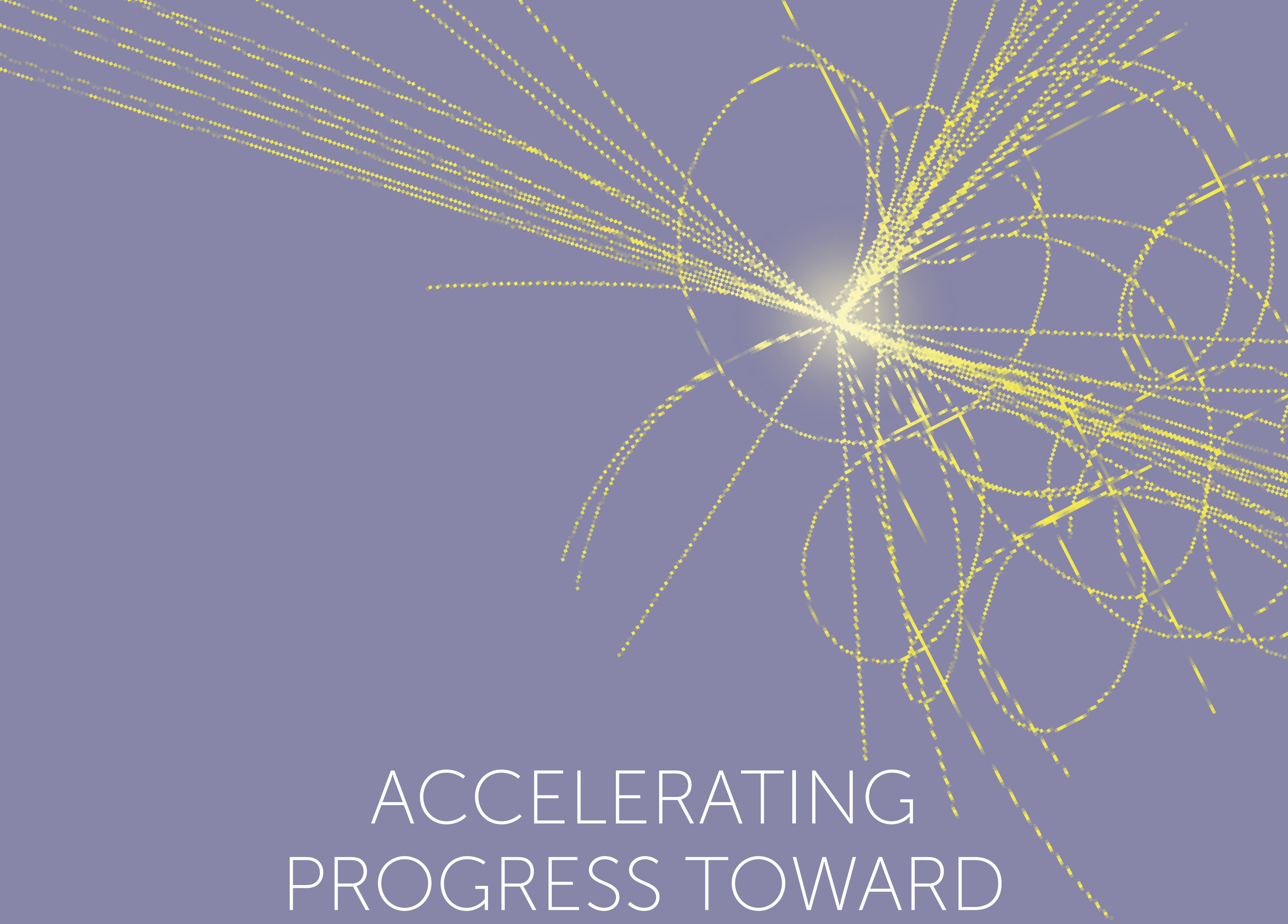
As discussed in Sections 3.3 and 3.4, there can be an inverse relationship between the level of a fabrication technology and the difficulty of designing and modeling the components and systems that it can produce. In AP nanosystems, several basic directions of progress lead not only to better products, but to reductions in engineering difficulty. Each of these remedies difficulties of working with biopolymers and derived materials:

- Materials that are more stable and fine grained.
- Functional components that are higher performance and more diverse.
- Direct control of the placement of parts during assembly

Projections of the pace of technology development are always highly uncertain, but it does seem clear that advances along this development path will facilitate design and modeling, and thereby accelerate progress toward more complex and capable productive nanosystems. In this connection, it should be noted that with typical production processes of the sort discussed here, the delay between completing a design and having a testable product is likely to be measured in minutes or hours, not months or years.

nano

Nano-solutions for the 21st century



ACCELERATING PROGRESS TOWARD ADVANCED NANOTECHNOLOGIES

4

4. Accelerating progress toward advanced nanotechnologies:

Guiding Technology Development

Many challenges in developing next-generation nanosystems, and atomically precise nanosystems in particular, are at the level of specific areas of science and technology. These are outlined elsewhere in this report, and in its companion document, the Battelle/U.S. National Labs technology roadmap for productive nanosystems and atomically precise manufacturing.[1] There are, however, challenges at another level: The level of organization and management that guides the development of these areas of science and technology, and helps them to move toward high-payoff objectives with relative efficiency and speed.

These resulting challenges are generic, not specific to nanotechnology, because they arise from the general problems in building complex heterogeneous systems, of coupling scientific research to engineering development, of integrating areas of research that have been separate, and of developing institutions and policies that can meet these challenges.

In nanosystems development, specialized and largely academic scientific disciplines are converging to develop the technology base for a new kind of systems engineering, one that, in turn, can support the further advances in AP nanotechnologies that can enable the development of high-throughput atomically precise manufacturing.

Nanosystems development presents the generic problems in a clear and prominent way, prompting questions about potential responses that have broader applications to areas of emerging technology and complex system development. This section and the next outline and describe aspects of technology development that are familiar in essence because they are so universal. Accordingly, most of the discussion is organized around universal problems and responses to them. At every point, what is said about the challenges of developing new systems applies strongly to developing nanosystems, and usually applies even more strongly to developing AP nanosystems.

4.1. A New industrial revolution: new opportunities and challenges for society

Because of the nature of the task, accelerating progress toward advanced nanotechnologies will require a review of existing institutional structures. Accelerating progress in this broad sense means developing an increasingly advanced technology base—a technology base that enables the development of increasingly complex nanosystems built from increasingly high-performance components and materials, and that enables engineering of systems on an increasingly routine basis for a growing range of applications. The emergence of these capabilities would be a natural consequence of prolonged, uncoordinated, incremental progress, but a more focused effort could accelerate progress, reduce costs, reduce risks, and deliver critical problem-solving applications at an earlier date.

The nature of the task differs because it is at a higher, more general, and more strategic level. The aim is not to develop products for some specific application, but to develop a technology base that enables the development of increasingly advanced products with an increasing range of applications.

Any advanced and broadly applicable technology base (whether it be for aerospace systems, optical instruments, or semiconductor fabrication) will be complex: It will rely on and integrate diverse materials, components, instruments, and tools, and will rely on and integrate diverse techniques for design, fabrication, and testing. Because of this, the task of coordinating research to drive a technology base forward into new territory presents challenges to managers and policy makers as they attempt to judge the utility of competing proposals for new developments.

This is particularly difficult because the value of each development will depend on the context of other next-generation technologies. Judging this value is critical: To develop sets of next-generation technologies that work together requires that research managers share an understanding of that next-generation technology context, and success requires that, in each of many areas, managers are working to create the technologies that will, together, create that technology context. This coordination process is best exemplified by the semiconductor industry, and it has been the basis for swift, exponential progress.

Establishing, managing, and coordinating research programs of this breadth presents multiple challenges. These include:

- Integrating cross-disciplinary research
- Identifying high-value applications and their requirements
- Managing research to fulfill requirements and achieve objectives
- Developing institutions organized for nanosystems engineering

Opportunity:
Integrating cross-disciplinary research

Nanosystems will incorporate a great diversity of materials and components, and will make use of a wide range of physical phenomena in their operation. This calls for simultaneous progress in diverse areas of applicable nanoscience and nanotechnology. Each area must focus on objectives that support system building capacity, but a great portion of the necessary research can be adequately coordinated by means of general standards for assessing progress, as discussed in greater detail in Background section B4. Closer direction and coordination will be required when specific systems are under development, because these will require compatible components that meet design specifications.

Opportunity:
Identifying high-value applications and their requirements

Effective application-oriented research requires the identification of achievable objectives and the requirements for achieving them. To do this effectively requires engineering design and analysis at a level appropriate to assess concepts: to identify principles of operation, workable combinations of components, and the general requirements that those components must satisfy. The closer the concept is to implementation, the more specific the design and analysis, but even an advanced and speculative concept can be explored in a quantitative way and at the level of functional parts. This process of exploratory engineering assessment is necessary to avoid research that cannot possibly achieve the proposed result, and to avoid the risk that a valuable application will be thwarted because of a failure to recognize and develop necessary parts.

Opportunity:
Managing research to fulfill requirements and achieve objectives

To be effective, a research program for developing nanosystems must express requirements and objectives as a basis for selecting research proposals and evaluating research results. This can be accomplished by means of criteria and metrics developed through exploratory engineering assessment. In conventional engineering, the fundamental nature of components and systems is well understood, and fundamental criteria and metrics are often implicit. In the present stage of development of nanosystems engineering (and of AP nanosystems in particular), new phenomena, new devices, and new kinds of systems all increase the difficulties of defining and judging research objectives, proposals, and results. The ongoing development and application of criteria and metrics can make this process more explicit and transparent, can make research more effective, and can make the achievement of ambitious objectives more practical and lower risk.

SIDEBAR 8

Research in China: the Science Citation Index metric

According to a 2005 study of the scale and impact of science in China,

"In the past ten years, universities and research institutes in China adopted the SCI [Science Citation Index] as the main indicator for research evaluation, and simply equate SCI-CPs [SCI-indexed Chinese papers] with high quality papers. Subsequently, a competition in the number of SCI papers started across all organizations. Moreover, various incentive measures were taken, one of which is to give special rewards to SCI papers: the more papers indexed by Thomson-ISI are published, the higher the reward for the institute or research group, sometimes even for the researcher herself. The immediate result of this policy was that the energy of Chinese scientists became focused towards publication in ISI-covered international journals."[62]

The application of this metric has proved fruitful in increasing both the quantity of scientific research output and the quality of the output, as measured by citations in other scientific papers. However, this metric also induces Chinese researchers to adopt research priorities set by scientists in other countries, and those priorities may not be well-aligned with Chinese needs, and are often not well-aligned with solving technological problems.

Quantitative metrics that can be related to technological problems offer an alternative approach to the problem of transparent and objective assessments of research progress that could potentially provide a useful supplement to counts of the number of papers produced.

Opportunity:
Developing institutions organized for nanosystems engineering

Today, most research in nanotechnology is organized on the model of scientific exploration and discovery. This is well suited to discovering new phenomena and new structures, and this task continues to be necessary and valuable. However, progress of this kind can only enable—not achieve—the development of complex systems. The next stages of nanosystems development will require the design and production of compatible functional components and the development of means for organizing and joining them to build complex structures. In addition, progress will require the development of design methodologies adapted to the physical principles and fabrication technologies in this area. Experience has shown that tasks of these kinds are best conducted in institutions that are organized to undertake the engineering of complex systems. These differ from institutions organized to promote scientific exploration and discovery. Both kinds of institutions will be necessary to ensure robust progress as nanotechnology moves deeper into the system-building era.

SIDEBAR 9

Example: Advancing a basic enabling technology

Synthesis of nanoparticles and nanocrystals has been an area of strength from emerging countries. For example, in 2005 in China, researchers working in this area at Tsinghua University published a paper in the journal Nature that exemplifies the concept of advancing a basic enabling technology—that is, a technology that is important, not for contributing to a specific application, but for enabling a spectrum of applications.[91]

In their paper, "A general strategy for nanocrystal synthesis", the authors describe means for producing diverse functional components with applications in equally diverse self-assembled materials and nanosystems. The authors note that "New strategies for materials fabrication are of fundamental importance in the advancement of science and technology", and they report a method with remarkably wide scope:

"...a unified approach to the synthesis of a large variety of nanocrystals with different chemistries and properties and with low dispersity; these include noble metal, magnetic/dielectric, semiconducting, rare-earth fluorescent, biomedical, organic optoelectronic semiconducting and conducting polymer nanoparticles."

"We believe our methodology provides a simple and convenient route to a variety of building blocks for assembling materials with novel structure and function in nanotechnology."

As of September, 2009, the paper has garnered over 290 citations. Many "citation classics" in science are papers that report the development of enabling technologies.[92]

4.2. Ways to capture the opportunities

The following sections discuss criteria and metrics, exploratory engineering, and technology roadmapping as a complementary and mutually supportive set of activities that can capture opportunities to developing next-generation, system-level nanotechnologies. In brief:

Exploratory engineering identifies and analyzes potential high-payoff system-level development objectives.

Criteria and metrics define the kinds of components required to build a system, and the characteristics of those components that determine system-level performance.

Technology roadmapping brings experts together from groups in multiple fields to examine the status of the technologies necessary to fulfill the system-level requirements for various potential objectives, and to develop shared plans and expectations for how research and development will proceed. Technology roadmapping can be applied on many levels.

Each of these has additional roles, as discussed below.

4.2.1. Directing research through physical criteria and metrics

As discussed earlier, parts of research in nanotechnology have been prone to inflated claims and to seemingly useful results that do not find their way into use. This suggests the need for better and more systematic ways to relate research to applications, and to measure progress toward useful results.

Physical criteria and metrics perform a ubiquitous function

In engineering, physical, application-oriented criteria and metrics are ubiquitous. Metrics describe performance properties: the strength of a material, the power density of a fuel cell, the switching speed of a logic gate, and for almost anything, generic properties such as mass and maximum operating temperature. Criteria are also ubiquitous, and the most fundamental criteria are the ones that distinguish between devices of different kinds: A wheel isn't a bearing, and a bearing isn't a motor.

In applied research, where the aim is to develop research products (components, systems, processes) that will be useful in some engineering application, the criteria and metrics for that application define the conditions for success. In the frontier areas of nanotechnology, however, criteria and metrics are often ignored, and are sometimes replaced by grand, unsupportable claims. A molecule that cannot possibly serve as a gyroscope is called "a molecular gyroscope", a molecule that cannot possibly serve as a digital logic component is called "a molecular AND gate",[60] and so on.

It is important to recognize that the function served by physical criteria and metrics is inherent in any effort to develop a new technology. In any development effort, there is always some understanding of what properties will be valuable. If these ideas are not examined, they may be inferior, misleading, biased, or incomplete. Explicit exploratory engineering is valuable because it can produce better and more concrete development objectives, and because it can produce a better and more complete understanding of what will be required, and how different results can contribute.

Physical criteria and metrics are broadly applicable

More widespread and systematic application of physical criteria and metrics would provide a common basis for comparing different proposed solutions to engineering problems, and would provide a basis for decreasing the misallocation of attention and resources caused by false claims of utility.

Physical criteria and metrics can and have been applied to all levels of systems and all stages of system development. In the data and organization of engineering catalogs, they are applied devices and systems that are already in physical existence. In semiconductor manufacturing roadmaps and in aerospace systems engineering proposals, they are applied to proposed systems that are years and billions of dollars away from implementation. In the roadmap for quantum information processing,{c61} they are applied to assess and compare extraordinarily diverse physical systems with respect to their research promise. Thus, they can and are applied to systems that are in the stages of theoretical study, conceptual development, and engineering analysis. They can be applied to design concepts that are very detailed, or that are very abstract.

In exploratory studies, of course, the level of confidence in a result will depend on the quality of the available information and analysis. However, even a very approximate exploratory analysis can divide concepts into (1) those that are clearly unworkable, (2) those that are clearly attractive, and (3) those for which further study or experimental research is needed before they can be reliably assessed. In group (3), the exploratory analysis can indicate important questions to study. Thus, criteria and metrics can help both to evaluate and to guide research.

Physical criteria and metrics can help orient research and research investment

To implement the use of physical criteria and metrics to evaluate research objectives and progress, research proposals must describe the anticipated results of success, in terms of the potential characteristics and performance of the resulting products or processes. The application of criteria then can indicate whether a promised or achieved result might be useful in the context of the overall purpose of the research program, while the application of metrics can be used to measure improvements, and sensitivity analysis can be used to judge the relative value of improvements of different kinds. On a larger scale, metrics can provide a transparent and objective basis for incentives and program review.

There are, of course, many other considerations that must enter into assessments of research programs, proposals, and results. These include the cost of the research, the likelihood of success, the value of pursuing multiple approaches to solving a problem, the value of research that can serve multiple purposes, and the possibility of surprising and useful discoveries. The value of applying criteria and metrics as a basis for assessment varies from high to low along a spectrum of research activities that reaches from engineering development to basic science.

4.2.2. Finding directions through exploratory engineering

Exploratory engineering develops and analyzes concepts for useful systems before the means for implementing those systems have been developed. Early in research, these concepts may be very general, and the analysis very approximate; closer to development, exploratory engineering transitions smoothly into product engineering, where concepts are reduced to detailed designs, and analysis becomes more exact.

Like all engineering activities, exploratory engineering explicitly or implicitly develops functional criteria for components and processes when describing the structure of a system, and it explicitly or implicitly develops and applies metrics when analyzing the system. Useful physical criteria and metrics correspond to system-level requirements and the characteristics of components that determine system-level performance. Exploratory engineering is thus tightly linked to the development of criteria and metrics; it also serves an initial surveying function in the development of technology roadmaps that lead to innovative destinations.

Exploratory engineering systematizes a ubiquitous function

It is important to recognize that, as with physical criteria and metrics, the function served by exploratory engineering is inherent in any effort to develop a new technology. In any development effort, there is always some idea of what is being developed, and some idea of what specific results will contribute to a successful outcome. If the underlying design concepts are not examined, they may be impossible, surprisingly difficult, or far from optimal. Without a design-oriented process, requirements may be overlooked or misjudged.

Explicit, competent exploratory engineering can define complete sets of system requirements, and thereby draw attention to gaps in the existing technology base. Development and application of the corresponding criteria and metrics can reduce the likelihood of overall failure by identifying any specific, critical needs that have not yet been met, and by providing measures of progress that can be the basis of planning, incentives, investment, and organization. Without exploratory engineering, criteria, and metrics, it is difficult to establish a systematic way to identify what must be done, and to recognize when it is done well.

Exploratory engineering can be applied in areas of highly uncertain scientific knowledge

When an area of science and technology is at a very early stage, exploratory engineering should recognize and accommodate enormous uncertainty regarding potential research results. The process may yield only approximate descriptions of potential applications, and general descriptions of what may be required, and convey great uncertainty regarding whether or not a useful result will be possible. An optimistic estimate of the unknowns may say yes, while a conservative estimate will often say no.

Even in these circumstances, the results of explicit exploratory engineering may be of great value. The results of the exploration may suggest new objectives that are highly valuable or more achievable. The engineering analysis may make requirements more complete and concrete. The recognition of uncertainties and their role in potential applications may help research groups to focus on the critical questions, seeking answers that will improve confidence or lead to reevaluation of the relative value of different lines of research. These contributions are of kinds that can reduce the costs of fruitless research, the risk of failure, while increasing the likelihood of recognizing rewarding opportunities.

It is often said that a field is not yet ready to support an engineering analysis, because more knowledge is necessary. This is true only if the concept of "engineering analysis" is restricted to production-oriented engineering. In any form of applied research, however, consideration of means and ends is implicit. Exploratory engineering makes this consideration of means and ends explicit and transparent, even if the result of the analysis consists of more questions than answers.

Conservative exploratory engineering can be restricted to areas of established scientific knowledge

As discussed in Section B5, exploratory engineering can be performed on the basis of highly conservative assumptions and the provision of large error margins. The engineering process can choose designs that are optimized, not for their performance, or for their manufacturability, but for their simplicity and ease of analysis. This approach can be used to describe lower bounds on the performance of potential systems, with high confidence that the resulting standard of performance can be met and exceeded. This requires adherence to a very conservative constraint on the components and processes that are admissible in the designs, and this is the strict avoidance of poorly understood materials and phenomena. This stringent restriction enables modeling and design calculations in which bounded errors permit bounded error margins, enabling reliable conclusions at the expense of what may be large reductions in performance.

Conservative exploratory engineering enables the analysis of HT-APM

Conservative exploratory engineering can show that current scientific knowledge implies that a particular class of physically possible components and systems would, in combination, constitute a valuable technology base. Results of this kind are the basis for the current understanding of lower bounds on the capabilities of HT-APM systems. The physical principles of these systems and the nature of the physical analysis applied to them are discussed in Sections B3 ad B5. These principles and methods are familiar and well-understood.

Because atomically precise products and processes are well defined (they normally have no stray molecules or unpredictable variations), the problems of computational modeling are greatly reduced. As a consequence, an exploratory engineering analysis can be applied with confidence to a range of production processes. The results support the assumption that a wide range of high-performance components and systems can be fabricated — and these products include the production systems themselves. In HT-APM technology, very conservative design rules indicate a lower bound on performance that is, by current standards, extraordinarily high.

4.2.3. Integrating research through technology roadmapping

A technology base for complex systems (whether these are aerospace systems, digital logic systems, or nanosystems) consists of many diverse technologies that are complementary: They are compatible, serve different functions, and in combination, they enable the design and fabrication of complex, heterogeneous products.

Effective roadmapping processes develop realistic, shared expectations for the state of a set of complementary technologies at a series of times in the future. Realistic expectations may include considerable uncertainty, but roadmapping can often raise expectations and reduce uncertainties. Further, it can share this improved knowledge among all the groups responsible for developing the set of complementary technologies that, together, will expand the scope and raise the level of the technology base. This can coordinate development, reduce costs, reduce risks, and sometimes greatly accelerate the achievement of useful results.

Roadmapping processes are diverse in methodology, purpose, and scope,[65–67] and have been applied in diverse areas. Areas within nanotechnology, in particular, have been the focus of multiple roadmapping projects sponsored by governments[68] and industrial groups.[69]

Roadmapping systematizes a ubiquitous process: the development of coordinated expectations regarding future technologies

In every area, there are expectations regarding future technologies, and from the perspective of a research and development manager, some of these future technologies—the ones that contribute to an overlapping technology base—are either competitive or complementary. Uncertainty about potential competitors creates risk, and causes a pressure toward high performance and fast development. Uncertainty about complementary technologies, however, creates a different kind of risk, because new, high-performance technologies will be useful only if the required complementary technologies also exist.

Roadmapping can speed progress and reduce waste

The semiconductor industry is famed for its smooth and rapid advance, as measured by metrics such as device size, memory size, and computing capacity. This requires many coordinated developments, and these are facilitated by an ongoing roadmapping process: the International Technology Roadmap for Semiconductors (ITRS).[63]

"...it is the purpose of the ITRS documents to provide a reference of requirements, potential solutions, and their timing for the semiconductor industry. This objective has been accomplished by providing a forum for international discussion, cooperation, and agreement among the leading semiconductor manufacturers and the leading suppliers of equipment, materials, and software, as well as researchers from university, consortia, and government labs."[64]

The ITRS creates shared expectations among researchers and producers in an enormously diverse range of technologies. This gives those in all areas confidence that their advanced products will enter a market with complementary advanced needs. It reduces effort that would otherwise be wasted in developing systems that are too far behind or ahead of the industry.

Roadmapping can remove roadblocks

In comparison to the semiconductor industry, the aims of advanced nanotechnology developments are more heterogeneous, and laboratory-level advances must rely on science that is less well understood. As a consequence, the appropriate level and methodology for roadmapping differs substantially from what we see in the ITRS. Roadmaps for advanced nanotechnologies must address questions of system-level development at a basic level, building a greater degree of consensus on objectives and concrete implementation strategies.

Nanosystems development today faces barriers between specialties and the lack of an ongoing systems-engineering culture and process. One consequence of this is unawareness of capabilities expected (or even those currently available) in other fields, and a consequent failure to develop other members of a potentially high-value set of complementary technologies. In effect, each can have confidence in the absence of complementary technologies, and will mutually fulfill this negative expectation.

In a roadmapping process, experts meet to discuss potential advances in their fields and how these can fit together to make systems that are more advanced, or entirely new. These meetings and discussions can create collaborations among participants, but more important, they can create widespread mutual expectations that enable advances that otherwise would never occur.

The ties between roadmapping and exploratory engineering are obvious. Exploring what can be done with future technologies is the purpose of exploratory engineering. Roadmapping is a process that can move a research community in some of the directions that have been explored. And roadmaps like the ITRS are, of course, engineering documents saturated with criteria and metrics.

4.2.4 Improving coordination and effectiveness through institutional policies

Nanosystems will become components of complex systems, and will themselves become increasingly complex. Managing this complexity requires managing a complex cooperative activity. This will require policies that develop a framework for effective coordination across a wide and diverse network of relationships that span multiple fields of engineering and multiple areas of scientific research. The activities outlined in the preceding three sections can be developed and applied through appropriate institutional policies. They are applicable to this vast coordination problem, and are mutually supportive:

Coordination through criteria and metrics

As discussed in Background section B5, physical, application-oriented criteria and metrics can be used to improve coordination across multiple disciplines, and can be used to more closely link the very different activities of scientific inquiry and engineering design. Their application can also increase research efficiency by screening out proposals that cannot possibly produce a result of the kind that is promised, and can enable more objective and transparent assessments of proposals and results at both the project and programmatic levels.

This indicates the value of implementing processes for developing criteria and metrics for research areas, and for incorporating them into the preparation and evaluation of research proposals and research reports.

Coordination through exploratory engineering

As discussed in Sections B5, exploratory engineering can help the research community develop new concepts and directions for research, can help to develop criteria and metrics for new and existing system-development objectives, and can help to ensure that all of the requirements for these systems have been explicitly and quantitatively described. By this means, exploratory engineering can reduce the risk of project delays that result from the neglect of necessary requirements, and can reduce the risk of project failures that result when a neglected but necessary requirement is impossible to satisfy.

This indicates the value of requesting that each development objective, even when in a very preliminary and approximate form, be described in the form of an explicit design and analysis, including the best current understanding of their implementation requirements.

Coordination through technology roadmapping

As discussed in Section B7, technology-base roadmapping can promote coordinated development in several ways. The roadmapping process can establish communication among groups that are developing complementary technologies, helping them to build a shared understanding of current knowledge and capabilities, and thereby highlight weaknesses that must be repaired, and strengths that can be shared. Further, it can enable them to jointly develop plans and shared expectations, and thereby enable them to gain greater confidence that bold advances by groups in one area will be supported by the necessary complementary developments in the others.

This indicates the value of establishing ongoing roadmap development processes that establish expectations (to the extent possible) regarding the development of complementary sets of technologies that, together, can raise and broaden the technology base for next-generation nanosystems.

Coordination of policies through institutional criteria and metrics

Unlike exploratory engineering and technology-base roadmapping, the concept of criteria and metrics generalizes beyond a technical context, and is applicable to institutions themselves. This is among the topics discussed in Section B7.

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Nano-solutions for the 21st century

Photograph courtesy NASA

POSSIBLE NEXT STEPS

5

5. Possible Next Steps

Global Collaboration in the 21st Century

The prospect of the emergence of deeply transformative new technologies for manufacturing changes the realm of possibilities for global development and global risks in the 21st century. It is important to consider these possibilities in order to formulate polices that respond to the opportunities and minimize needless risks.

When considering ordinary developments in technology, it is appropriate to evaluate how they would affect specific concerns and goals within the framework of established national and global interests. Deeply transformative developments in technology, however, can change the framework itself. It may therefore be necessary to begin by considering how the new technologies would change national and global interests, and then subsequently to consider their effects on specific concerns and goals as they would appear in that context.

A fundamental dimension of policy and human affairs is the balance between pressures for competition and pressures for cooperation. This balance affects across a broad spectrum of policies regarding economic development, military posture, and openness of research in science and technology. The prospect of HT-APM changes these pressures, and strongly favors cooperation in key areas.

5.1. Global competition for scarce natural resources is growing

Competition for scarce natural resources is a recognized source of international tension, and economic growth based on current technologies is widely expected to lead to intensifying struggle.

In its 2009 annual report on "The Military Power of the People's Republic of China", the U.S. Department of Defense states that "As China's economy grows, dependence on secure access to markets and natural resources, particularly metals and fossil fuels, has become an increasingly significant factor shaping China's strategic behavior."[70] In a 2008 statement to the U.S. Congress, the Chairman of the Joint Chiefs of Staff listed "a growing global competition for scarce natural resources" as a potential threat to vital national interests.[c71]

A white paper from the Information Office of China's State Council, "China's National Defense in 2008", states that "... factors conducive to maintaining peace and containing war are on the rise, and the common interests of countries in the security field have increased, and their willingness to cooperate is enhanced, thereby keeping low the risk of worldwide, all-out and large-scale wars for a relatively long period of time.", but also states that "Struggles for strategic resources, strategic locations and strategic dominance have intensified....",[72] and in 2006 referred specifically to security issues related to energy and resources.[73]

David King, former chief scientific adviser to the British government, suggests "that future historians might look back on our particular recent past and see the Iraq war as the first of the conflicts of this kind—the first of the resource wars".[74]

A transformative change in production technology can avoid this future, and thereby remove a major challenge to harmonious global development. The characteristic advantages of HT-APM—precise control of material structure, inherently high productivity, and the resulting low cost of production—can be applied to reduce (and in some instances eliminate) the conflict between global development and shrinking supplies of scarce raw materials and fossil fuels.

5.2. Competition for scarce resources can be greatly reduced

Ending dependence on fossil fuels

Energy, including energy-dense vehicular fuels, can be provided from solar sources together with efficient means of inter-converting electrical and chemical energy. At the same time and even more important, energy demand can be dramatically reduced by improving the efficiency of vehicles, lighting, thermal insulation, and other areas, including industrial production. Demand reduction and abundant renewable sources of carbon-free fuel and solar electric power can enable global development that is sustainable with respect to both energy supply and greenhouse gas emissions, and at the same time can reduce competition for globally scarce energy resources.

Reducing demand for fuels: In transportation, energy demand can be reduced by reducing vehicle mass through stronger materials, and by increasing energy-conversion efficiency through improved batteries, fuel cells, and motors. Improved thermal insulation and more efficient lighting can reduce home energy requirements. Improvement in ICT technology will allow more physical transport to be replaced with virtual meetings and decentralized production can significantly reduce the need for physical transport over long distances.

Replacing fossil fuels with solar-derived energy: Low-cost, high-efficiency products could be used to implement a synergistic, carbon-neutral chain of energy conversion systems:

- From solar energy to electrical energy
- From electrical energy to energy-dense fuels
- From energy-dense fuels to electrical and mechanical energy

This technology infrastructure can support industrial, home, and vehicular energy requirements. Simultaneously, deployment of systems with these capabilities can end dependence on fossil fuels, and with this, can end scarcity-driven conflicts over access to petroleum.

Conserving and replacing scarce raw materials

As another consequence of precise control of material structure and inherently high productivity, HT-APM production systems can reduce resource requirements and enable extensive substitution of materials.

Precise control of material structure through HT-APM can enable the production of high-performance materials that reduce the demand for scarce resources in two ways: by requiring less mass to perform common functions (architectural and mechanical structures, electrical conductors, electronic systems...), and by enabling the use of abundant elements (hydrogen, carbon, silicon, oxygen, aluminum...) in most applications, substituting them for scarcer materials (copper, nickel, cobalt, gallium...). Products of HT-APM could also enable economical extraction of metals from recycled waste streams, and from dilute sources, rather than scarce, concentrated ores. These measures can further reduce the level of demand and competition for globally scarce raw material resources.

More performance from less material: Resource requirements can be reduced because of increased performance per unit mass (improved strengths, power densities, and so on). In particular, the use of rare materials in catalysis (for example, platinum) can be greatly reduced by the two fundamental characteristics of HT-APM: precise control of processes at a molecular level can prevent the release and loss of catalytic materials, and can greatly increase the productivity of these materials (for example, in a nanoscale mechanochemical system operating at a nominal 10^6 cycles per second, a platinum atom in a catalytic center could process ~10^6 times its mass per second, yielding ~10^7 tons of product per year per gram of platinum).

Replacing scarce raw materials: Scarce materials can often be replaced because most critical engineering functions (electrical, mechanical, thermal, and optical) can be performed by materials made from combinations of common elements, such as carbon, hydrogen, nitrogen, oxygen, aluminum, silicon, and iron. Structural metals (and their alloying elements) can be replaced by stronger materials based on carbon fiber or fracture-tough ceramics; copper conductors and soldering alloys might be replaced by higher-conductivity quantum wires.[75]

Substitution of materials will be more limited, where properties depend on special electronic characteristics of materials, for example, superconductors, semiconductors, phosphors, and magnets. In some instances material substitution can be achieved by using an entirely different kind of device to serve the same purpose. For example, phosphors (many of which contain rare earth elements) are used chiefly in electroluminescent devices and for converting short wavelength light to longer wavelength light; advanced fabrication methods, however, can optimize light emitting diodes that produce the light at the desired wavelengths directly and more efficiently. For another example, high-performance magnets (which contain rare earth elements) are important chiefly in electric motors that operate by means of magnetic forces; scaling laws, however, strongly favor the use of electrostatic forces in small systems, and relative to conventional magnetic motors, nanoscale electric-field based motors can deliver enormously greater power density (Table B2a).

Improving recycling and extraction: Products of HT-APM could also enable economical extraction of metals from recycled waste streams and dilute sources, rather than scarce, concentrated ores. The principle involved is a staged-cascade system of concentrators using selective ion binding for transport across membranes; processes of this kind can be made thermodynamically efficient in nanomechanically coupled systems operating near equilibrium.[16]

5.3. Adversarial development risks military surprise

Technologies at the level of HT-APM will greatly expand human capabilities. The technological results that can be predicted with confidence are large enough to ensure disruptive change, and the prospect of unpredictable technological developments creates further uncertainty. Technological disruption and uncertainty extend, of course, to military technologies, an area where disruption could lead to disaster.

The technology drivers for these changes include shifts by factors that range from tens to millions in feasible materials performance, energy-conversion power density, density and energy efficiency of computation, size of miniature components, cost of production, and rate of production scale-up. A few general examples should be sufficient to suggest the magnitude of potentially disruptive changes in military capabilities:

Advanced conventional systems

The above technology drivers can greatly increase the feasible performance of conventional-style weapon systems, the scale of their deployment, and the rate at which new designs can advance from final testing to large-scale production.

Miniature mobile systems

The potential for extreme miniaturization of sensors, computational devices, and electromechanical systems can enable the development of small systems with new capabilities: A mass of one gram is ample for implementing a complex, mobile, multi-functional device, and a ton contains one million grams. This will allow for powerful, fine-grained, networks of sensors, actuators, and communication devices.

Pervasive and non-lethal systems

Potential capabilities resulting from the above include extensive surveillance and more controlled application of coercive force. Non-lethal weapons will become more practical as their production costs fall and their capabilities increase, potentially lowering the threshold for initiation of aggression.

Military history suggests that changes of this magnitude can cause surprises, mistaken assessments, and unwise actions for several reasons:

- Unexpected military applications of new technologies
- Overestimates and underestimates of the effectiveness of new technologies
- Uncertainty regarding a competitor's current and emerging capabilities
- Slow responses of institutions to new information

The transition ahead can be expected to cause each of these problems, not once, but many times, in many areas. Errors of judgment and action are inevitable, and in an adversarial context, these errors would have unpredictable consequences of potentially enormous magnitude. (See also Section B6.)

5.4. Cooperative development can reduce risks

A competitive arms race during this technology transition, in the midst of other turbulent and unpredictable change in the global environment, would present grave national and global risks. The alternatives to competition are cooperative development and unilateral dominance. Both paths present risks, but in the present instance, multiple considerations indicate that cooperative development is by far the less risky course.

The transformative potential of HT-APM in the military sphere, as with all powerful technologies, will inevitably lead to unexpected consequences and misinformed decisions. In an adversarial environment, the consequences could include strategic instability and outcomes that place national and global security at risk.

In considering the development and capabilities of HT-APM and its products from a military perspective, it is natural to consider parallels to nuclear arms. A detailed comparison with nuclear arms can provide a useful perspective: Both areas involve technologies of great strategic importance, but their differences are enormous and informative. This comparison is presented in more detail in table B6.

In outline, the development of nuclear weapons technologies is a well-understood, large-scale task that employs special equipment and materials to develop productive capacity, and this capacity is then used to make distinctive, well-understood products: Nuclear explosive devices. For many decades, advances in nuclear weapons technologies (both production processes and products) have been incremental and unsurprising in a strategic context.

By contrast, progress toward atomically precise manufacturing is proceeding along many paths, with both expected and unexpected advances. New developments have employed ordinary materials and laboratory-scale equipment. Current and expected near-term results are incremental, but developments are moving toward a scalable production technology able to make a wide and largely unexplored range of products that have a correspondingly wide and largely unexplored range of potential military and non-military applications.

In an adversarial context, these characteristics create unprecedented difficulties of predicting development paths, observing progress, and assessing an adversary's potential capabilities and options. Potential threats reach the existential level. For these and other reasons (Table B6), proceeding along a competitive and opaque development path appears to create risks that are large and incalculable.

These considerations strongly favor policies that lead to extensive, transparent, multilateral, laboratory-level collaborative development of technologies moving toward HT-APM. These policies of deep collaboration could offer several benefits:

- Deep, multilateral collaboration can provide a basis for building multilateral confidence.
- Open, visible progress can reduce tensions created by outmoded fears of future resource scarcity.
- Multilateral collaboration and confidence can provide a basis for working together to stabilize economic and social development.
- Combining global research contributions can accelerate progress toward toward rapid, clean, and sustainable global development.

5.5. Embracing opportunity and minimizing risk

Nanotechnology today includes many forms of atomically precise fabrication. Ongoing progress across many fields is converging to create a technology base for increasingly advanced atomically precise nanosystems with applications ranging from energy to medicine to advanced electronics. At a research-program level, there are low-cost policy options that can better exploit the near-term potential of atomically precise systems engineering, and do so within the framework of existing program objectives.

A broader perspective shows that progress in atomically precise systems engineering is opening paths to high-throughput atomically precise manufacturing. This advanced technology can be reached through a series of incremental improvements in atomically precise fabrication. As this level of technology is achieved, it can provide a basis for advances in many areas of technology by multiple orders of magnitude. This line of development was the basis for the original promise of nanotechnology as a transformative revolution in production technology, and it can fulfill that promise.

This picture of future capabilities differs from conventional expectations, and it is also better supported by current scientific knowledge. Conventional expectations rely chiefly on projections of trends and on speculation about the practicality of poorly understood future technologies: There is no reliable way to validate information of this kind. By contrast, expectations regarding the general capabilities of HT-APM and its products result from the application of engineering and physics-based methods of analysis. This kind of analysis establishes lower bounds on the capabilities of a limited class of well-understood physical systems. The resulting information can be validated and refined by means of rigorous methodologies based on scientific knowledge and well-known physical principles.

The expected capabilities of HT-APM naturally lead to deep, pervasive, transformative advances in production technologies, products, and general technological capabilities. These capabilities can provide a basis for accelerated and sustainable global development and steeply declining competition for scarce energy and material resources.

Personal, societal, and global relationships are closely linked to patterns of work, trade, wealth, and economic organization. Each of these patterns is shaped by the material basis of modern civilization, which in turn is based on current means of production. A great increase and qualitative change in production capacity can be expected to lead to cascading changes affecting all areas of human life and civilization.

It would be naïve to assume that a great and disruptive increase in the ability to provide for human needs will necessarily produce favorable results. Preparation for developments of this magnitude will require policies that begin with a rethinking of the future, and how transformative developments in technology will change national opportunities, risks, and objectives.

There are multiple implications. Prospects of declining competition for scarce resources can decrease the motivation for competition and conflict. The pressures of environmental degradation, climate change, and global poverty provide motivations for cooperation to accelerate the development of technologies that can accelerate sustainable global development. The risks of economic, social, and military disruption during a transition of this kind are enormous, and can be mitigated by policies that support deep, broad, transparent, international cooperation. These policies could accelerate development of peaceful and stabilizing applications, and could also provide the extensive international transparency necessary to implement agreements that can reduce the risks of disruptive change.

Policies informed by science must consider the implications of science-based engineering studies of the potential of future atomically precise manufacturing. Existing studies[1,16,79] can be assessed and extended, and their technical conclusions can be used as a basis for scenarios of investigation, technology development, and contingent policy responses. Incorporation of this information into national planning will be essential to the formulation of rational, science-based policies. Needless delays in developing and providing this information could result in needless national and global risks. Effective progress, by contrast, could accelerate solutions to what may be the greatest challenge of our time in history: The challenge of resolving the conflict between global environmental limits and accelerating global development.

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BACKGROUND SECTIONS

6

B1. Converging technologies: Application examples in photonics

The development of nanotechnologies is characterized by a convergence of enabling technologies that support development in multiple application areas. Within each area, there are typically multiple implementation approaches at various stages of development.

These relationships can be illustrated by examples from the development of solar photovoltaic and LED lighting technologies, both of direct importance to providing energy-based services, and by examples from the development of productive nanosystems, which are both products and enabling technologies for other products (Table 4).

Photovoltaic and LED technologies are related because both require transport and conversion of energy in optical and electronic forms. Device efficiency depends on structures and phenomena on multiple length scales:

• Atomic level	Crystalline order, defects, surfaces, molecular structures
• 1–10 nm	Geometry of quantum dots, wires, and wells
• > 10 nm	Organization of layers, wires, quantum dots
• >>1000 nm	Devices, packaging, products

Photovoltaic cells for solar electric power

Table B1 lists some of the classes of photovoltaic cells in use or under investigation, and some of the processing techniques that are necessary or potentially useful in making them.

Conventional crystalline cells, like most most classes of thin-film cells, are not considered nanostructured. They dominate the market today, but are made using expensive methods, such as batch processing under vacuum conditions.

Printed thin film cells are made using low-cost roll-to-roll deposition processes operating at atmospheric pressure. Looking forward, suitable self-assembling nanostructured materials would also be suited to roll-to-roll deposition processes.

Quantum-dot sensitized cells use quantum dots to absorb light and transfer electronic energy to a nanoparticle-based titanium dioxide electrode. PV cells of this class promise reduced fabrication costs. The size and composition of the QDs determines the light wavelengths that are absorbed, enabling adjustment to fit the solar spectrum.

Fabrication of QDs draws on multiple areas of chemistry, nanoparticle synthesis, and surface science. Linking QDs to electrodes draws on simple self assembly techniques. Looking forward, progress in Level 3 PNs will enable production of improved QDs, electrode-forming particles, and self-assembling linking structures.

Self-assembled-nanostructure cells would draw on more advanced self-assembly techniques to bind quantum dots to quantum wires that are aligned and linked to form low-resistance paths to current collecting electrodes, with advantages in device efficiency. Suitable self-organizing properties would enable these organized structures to be deposited by spray-on coating processes.

This self-assembly capability may draw on biomolecular engineering (based on Level 2 PNs), and would benefit from Level 3 capabilities. The active components (QDs and QWs) will draw on advances in synthesis of nanoparticles and nanorods; these advances will be extended by Level 3 capabilities, enabling more precise structural control of a wider range of electronic materials.

Multiple energy level cells are an alternative to multi-layer tandem cells for increasing the efficiency of use of a wider range of the solar spectrum, providing an advantage by being less sensitive to changes in the spectrum during the day. The most attractive kind of structure would consist of a highly regular self-assembled array of quantum dots, drawing on technologies for self-assembled-nanostructure cells.

Optimized-nanostructure cells made using advanced-generation PNs will use abundant, non-toxic materials such as FeS_2 (which occurs as the mineral pyrite) as a photovoltaic absorber in QDs and carbon in QWs. This contrasts with the scarce and often toxic materials used in most advanced cells now under development. PN-based fabrication will enable these to be combined in optimized structures of essentially perfect regularity and precise control of interfaces and band structures. The result will be high-efficiency photovoltaic systems (potentially approaching the theoretical limit of ~68%) with low mass, short energy payback times, and scalable to the terawatt scale necessary for global energy supply.

LEDs for high-efficiency lighting

Table B1 also lists some of the classes of light emitting diodes in use or under investigation, and some of the processing techniques that are necessary or potentially useful in making them.

Conventional crystalline LEDs today are more efficient than fluorescent lights, and as of 2009, they have found niche applications and are expected to soon be competitive in wide-spread use.

Photonic crystal enhanced LEDs use a nanostructured layer above a crystalline LED layer to improve the extraction of light. These can be made using semiconductor-style processing or self-assembly.

QD/polymer LEDs promise to reduce the cost of materials and fabrication by replacing semiconductor crystals with a material that contains QD light emitters in a conductive-polymer matrix. The use of QDs of multiple sizes can enable direct production of white light with increased efficiency.

SA-nanostructure LEDs would exploit technologies like those required for SA-nanostructure PV cells, with similar advantages in path resistance and use of efficient QD photonic structures that emit at multiple wavelengths.

Optimized-nanostructure LEDs will have advantages like those of optimized-nanostructure PV cells, including the use of abundant, non-toxic materials and optimized structures enabling high efficiency.

Broader convergences

Technologies for photovoltaics and LEDs are closely related to other photonic technologies such as optical sensors, fluorescent biosensors, and luminescent displays. Technologies for QD fabrication and self-assembly have potential applications in nanoelectronics, high-density digital memories, and targeted therapeutic nanoparticles. Fabrication techniques based on advanced-generation PNs will support all of the above applications by providing a new range of components and means for assembling them.

Table B1: Converging technologies. Solar photovoltaics and LED lighting share multiple nano-enabled materials and photonics technologies

Functional class	Current level of development	Characteristics (nonexclusive)	Semiconductor processing	Nanoparticle, rod (etc.) synthesis	Self-assembly	Biological PNs (Level 2)	Post-biological PNs (Level 3)	Macroscale PNs (Level 4)
Solar photo-voltaics	4	Conventional crystalline	++					–
	4	Printed thin film		++		+	+	–
	3	QD-sensitized		++	++	+	+	+
	2	SA nanostructure		++	++	+	+	–
	2	Multiple energy level	+	++	+	+	+	+
	1	Optimized nanostructure						++
LED lighting	4	Conventional crystalline	++					–
	3	Photonic crystal enhanced	++	+	+	+	+	+
	3	QD/polymer		++	+	+	+	–
	2	SA nanostructure		+	++	+	+	–
	1	Optimized nanostructure						++

1 = Physical principles known
2 = Components demonstrated
3 = Systems demonstrated
4 = Products in use

QD = Quantum dot
SA = Self assembled
AP = Atomically precise
PN = Productive nanosystem

+ = Applicable
++ = Necessary
– = Supersedes

B2. The physical basis

of high-performance nanosystems

The typically high performance potential of APM products results from the high performance of their components. In many instances, high performance is a direct consequence of physical scaling laws and small component sizes (Tables B2a, B2b). Other high-performance capabilities are unique and result from molecular and quantum properties that can be exploited only by nanoscale or atomically precise devices (Table B2).

Table B2a: Scaling laws that are predicted by classical mechanics and approximately correct for mechanical devices on a scale >3 nm. Adapted from “Productive nanosystems: the physics of molecular fabrication”.[80]

Physical quantity	Scaling conditions	Typical magnitude	
Scaling as L^3:			
Volume	-	10^{-24}	m^3
Mass	*Fixed density*	10^{-21}	kg
Gravitational force	*Fixed density*	10^{-20}	N
Scaling as L^2:			
Area	-	10^{-16}	m^2
Applied force	*Fixed applied stress*	10^{-8}	N
Dynamical force	*Fixed speed, density*	10^{-15}	N
Mechanical power	*Fixed speed, stress*	10^{-9}	W
Scaling as L^1:			
Length	-	10^{-8}	m
Stiffness	*Fixed modulus*	10^{3}	N/m
Elastic displacement	*Fixed modulus, stress*	10^{-11}	m
Motion time	*Fixed speed*	10^{-7}	s
Gravitational stress	*Fixed density*	10^{-4}	N/m^2
Scale-independent:			
Density	*(Material property)*	3×10^{3}	kg/m^3
Young’s modulus	*(Material property)*	10^{11}	N/m^2
Speed	*(Design parameter)*	10^{-1}	m/s
Applied stress	*(Design parameter)*	10^{8}	N/m^2
Dynamical stress	*fixed speed, density*	10^{1}	N/m^2
Dynamical strain	*fixed speed, density, modulus*	10^{-10}	-
Scaling as $L^{-1/2}$:			
Thermal fluctuation amplitude (r.m.s.)	*Fixed stiffness, temperature (here, 300 K)*	2×10^{-12}	m
Scaling as L^{-1}:			
Acceleration	*Fixed speed*	10^{6}	m/s^2
Stiffness	*Fixed modulus*	10^{3}	N/m
Motion frequency	*Fixed speed*	10^{7}	Hz
Mechanical power density	*Fixed speed, stress*	10^{15}	W/m^3

Table B2b: Scale-based performance advantages enabled by nanoscale devices.

Device metrics	Ratio*	Corresponding system metrics
Electromechanical devices: results of scaling laws		
Energy device cycle frequency	~10^{6}	Power density of motors, generators and transmissions
Fabrication device cycle frequency	~10^{6}	Fabrication productivity (mass/second per unit mass)
Volume number density of fabrication devices	~10^{18}	Number density of product components
Electronic devices: results of scaling laws + scalable, post-silicon technologies		
Operation frequency	~10	CPU instructions per second
Operations per unit energy	~10^{6}	CPU energy efficiency
Area number density	~10^{2}	Memory size, CPU number (planar)
Number per chip-scale package	~10^{6}	Memory size, CPU number (stacked)

*Some combinations of performance improvements are constrained by trade-offs.

Table B2c: Special device properties enabled by nanoscale physics.

Component	Property	Benefits and applications
Quantum dots	New optoelectronic properties	More efficient lighting, photovoltaics
Quantum wires	High electrical conductivity	Greater range and efficiency of power transmission
Flawless-fiber composites	High material strength, toughness	Reduced resource consumption, vehicle weight
Nanostructured thermo-electric materials	High figure of merit (*ZT*)	Conversion of waste heat into electric power
Chemical catalysts	New chemical processes	Energy and waste reduction, new products and raw materials
Electrochemical catalysts	New electrochemical processes	Improved batteries, fuel cells, fuel production
Molecular sensing and action	Controlled biological interactions	Nontoxic eradication of viruses, bacteria, cancer cells
Surface superlubricity	Low friction, zero-wear surfaces	Functional nanoscale machinery and manufacturing

B3. The physical basis

of atomically precise manufacturing

The principles of operation of APM based on productive nanosystems are outlined in Table {t B3a}; a quantitative tutorial discussion can be found in the Institute of Physics journal, *Physics Education*.[80] It is important to note that biological productive nanosystems (for example, ribosomes) demonstrate each of these principles of operation. It is also important to note that anticipated HT-APM systems are entirely non-biological in composition (using high-stability engineering materials, not using hydrated biopolymers) and in their manner of organization (using specialized, highly deterministic mechanisms linked by conveyors and integrated to form macroscopic factory-style systems, not using the collections of stochastic mechanisms linked by diffusion that constitute microscopic biological cells).

Table B3a: The physical principles of operation of APM-based fabrication of nanoscale products.

Properties shared by biological and prospective artificial productive nanosystems
Nanoscale devices can bind both chemically reactive molecules and larger structures.
Nanoscale devices can position molecules with atomic precision relative to larger structures.
Positioning reactive molecules with atomic precision can extend a larger structure at specific sites.
Programmable devices can direct sequences of structure-building chemical reactions.
Programmed sequences of structure-building chemical reactions can build complex, atomically precise nanostructures.

Exploratory engineering of HT-APM systems

Understanding of lower bounds on the potential of prospective high-throughput APM is based on a conservative physics-based analysis[16] conducted by means of the exploratory engineering methodology (Section B5). As a necessary consequence of this methodology, the analysis rigorously avoids the use of novel or poorly understood physical structures or physical phenomena.

Lower bounds on system performance are derived from lower bounds on component performance. High system performance is a consequence of the nature of the design domain, and does not require non-conservative assumptions regarding any of the components. High system performance is chiefly the result of

1) High operating frequencies that follow from elementary mechanical scaling laws (see Table {t B2a})
2) Specific results regarding the molecular dynamics of suitably designed, atomically precise mechanical components and their interfaces
3) Specific results regarding mechanical stiffness and limitation of the frequency of defects due to thermal fluctuations.

The exploratory engineering research methodology has been applied to establish the functional parameters of a set of mechanisms that has been selected to enable high-confidence modeling and analysis by means of standard physics-based methods. In accord with the methodology of exploratory engineering, the molecular structures of these mechanisms are not designed to satisfy the stringent constraints of synthesis by presently available means. Although no use is made of new or poorly understood physical phenomena, these structures are not of a kind suitable for direct, near-term experimental development. These structures are instead among the potential products of more advanced fabrication technologies that will become accessible only at higher levels of the ladder of technologies.

In this analysis, a specific set of mechanisms was examined in order to establish lower-bound, parametric estimates of the performance parameters of a set of classes of mechanisms that is sufficiently comprehensive to implement the operations necessary to perform HP-APM. System-level engineering analysis shows that mechanisms of this kind can be organized as non-biological, factory-style systems that can process and combine a wide range of molecular building blocks to produce a wide range of non-biological materials, atomically precise nanostructures, and larger assemblies. These products include structures of the kinds necessary to implement factory-style systems of the same kind. This physical basis for this conclusion is summarized in outline in Table {t B3b}.

Table B3b: The physical basis of high-throughput APM-based fabrication of large products.

Physical characteristics of feasible HT-APM components, devices, and processes
Atomically precise nanostructures can implement components that provide a full range of ordinary mechanical functions: Motors, bearings, gears, conveyors, and so forth.
These component functions are sufficient to implement machinery like that found high-throughput assembly systems.
Chemical and intermolecular interactions can play roles like those of fasteners, and can bind and align surfaces to form atomically precise interfaces.
Assembly of small atomically precise components can therefore yield larger atomically precise components, and this can continue through micro- and macroscopic scales.
All operations above the molecular level are assembly operations (no molding, machining, casting, coating, etching, heat treatment, polymer curing, *etc.*).
Machine stiffness can limit the r.m.s. amplitude of thermal fluctuations sufficiently that, with ample design margins, error rates in assembly operations are < 1 per 10^{15}
Energy dissipation per molecule in assembly operations can be limited to a small multiple of the energy dissipation in conventional chemical processing of materials.
The natural operating speeds of mechanical devices are independent of scale, hence the natural frequencies of mechanical operations are inversely proportional to scale.
On a throughput per unit mass basis, the natural productivity of assembly machinery is proportional to the frequency of operations, hence inversely proportional to scale.
The size and frequency ratios of conventional manufacturing machinery in comparison to machinery based on atomically precise nanoscale components are, respectively, approximately $1 : 10^{-6}$ and $1 : 10^{+6}$.
The natural productivity of nanoscale manufacturing machinery on a per unit mass basis can therefore exceed that of conventional machinery by a factor of $\sim 10^{6}$.
In a full production system, throughput is limited by the speed of assembly of the largest (end-stage) components that result from convergent assembly of smaller components.
The natural productivity of a full APM system, from raw materials to products, is similar to the productivity (mass-based throughput) of final assembly operations in conventional manufacturing.

The broader physical and engineering analysis supporting the above indicates that necessary system-level constraints not mentioned above can be satisfied. These include providing means for power supply, cooling, feedstock flow, feedstock purification, binding of input molecules to mechanical components, component and molecular transport, matching of mass throughput at successive scales of assembly, provision of control signals, and fault-tolerance adequate to provide reliable system operation in the presence of background radiation and failures of nanoscale components.

B4. Assessing progress:
applications of criteria and metrics

The task of accelerating current nanotechnology and also adding a focus on a new technology base require a review of existing institutional structures. Developing AP fabrication technologies on the path to high-throughput APM differs from usual modes of development in science and technology. The objective is not a product or an application, but a diverse technology base able to support the fabrication of successively more advanced products of a wide range of different kinds. Within this broad area of development, however, the products that will be most important are those that contribute to improved fabrication technologies.

In addition, the task of extending the AP technology base is very science-intensive. Although advanced AP fabrication technologies will make design and implementation more direct and predictable, critical technologies today are severely constrained by the nature of current techniques. Many current generation AP fabrication techniques have unpredictable results, limiting the scope for systematic design. The techniques used to make the most complex atomically precise structures (thousands to millions of atoms) work with biomolecules: The results are becoming increasingly predictable, but the products by nature are constrained to be made of specific polymeric materials, and fabrication continues to be more experimental than it is routine.

AP fabrication techniques are often applications of discoveries made in the course of basic scientific investigations of nanoscale phenomena (examples include many chemical reactions, methods of material synthesis, and useful biomolecular functions). This history illustrates the value of scientific investigation that is only loosely directed toward specific applications, pursued in parallel with science intended to help satisfy specific technological requirements.

In more depth:

Directing research through criteria and metrics

Criteria and metrics for systems, components, and processes are ubiquitous in engineering practice: They are the basis for determining whether something can perform a function, and how it will perform.

Criteria and metrics can also be applied in research to provide a systematic and transparent way to assess research programs, proposals, and results, and to provide a way to report research results in a form that is a useful input to engineering design.

From the earliest stages of research, exploratory design methods can help to clarify the potential value of different research results, and can help to identify results that are critical to implementing specific working systems that solve problems. This information takes the form of criteria for the usefulness of research products, and metrics that assess their relative performance.

Establishing procedures for integrating criteria and metrics more deeply into the research and development process could be highly beneficial.

The sections that follow, B5, discuss these topics in more depth, and the last section presents two case studies of the application of criteria and metrics to research results that were advertised as being "molecular logic gates". In the first case, elementary criteria would have rejected this claim before the research was funded, while in fact, the claim was accepted by a series of journals. In the second case, the system meets the criteria, but its innovative nature forces revision of the metrics.

Criteria and metrics in conventional engineering

In an established area of technology, metrics and criteria are illustrated by the the data provided in engineering catalogs, and by the way that the catalog is organized. Basic, qualitative criteria determine where in the catalog a component will be listed—for example, if a small, rotating device consumes AC power and produces torque, then it meets the criteria for being listed among AC electric motors, and not as a DC motor, a bearing, or a wheel. An engineer working on a specific design will compare and select motors based on size, torque, operating temperature range, and so forth. Design-derived criteria determine whether a device has properties (metrics) that make it suitable for the specific use (for example, ample power, small enough size). Performance and cost metrics then help an engineer to rank the alternatives.

Criteria and metrics in research programs

A nanotechnology research program that is aimed directly at applications can be thought of as an effort to add new products to a section of an engineering catalog. To be successful, these products must meet the criteria for the section and offer a combination of metrics that is superior for some range of applications.

These conditions for success can help to define clear objectives for research. Research proposals can be judged by their potential contributions, whether direct or indirect, to developing systems that satisfy criteria and improve metrics, and results can be judged in the same way. Sometimes this method will produce an objective and transparent standard for comparing research efforts.

In more difficult conditions, where practical results are several steps removed from current research, criteria and metrics can still provide a framework that can clarify the problems that need to be solved, and can help distinguish between relevant and irrelevant results.

Criteria and metrics in technology base development

Criteria and metrics can describe the requirements that must be satisfied for a set of technologies to serve as an enabling technology base for a specific range of system-level technology applications. A description at this level may reveal gaps that show the need for targeted research, or may reveal inconsistencies that show that a research program cannot possibly achieve its stated objective.

Production of a functional system of a particular kind (for example, a computer) requires a technology base that can provide a set of components that collectively:

1) Are of mutually compatible kinds (as a familiar example, to produce electronic digital systems, a technology base must be able to produce devices that share compatible ranges of input and output voltage).
2) Serve all the necessary functions (for example, supply power, transmit signals, perform digital logic operations, and so forth).
3) Provide adequate performance (for example, provide sufficient power, fast enough switching, ample noise margins).

The conditions (1) and (2) are criteria for the functional coherence of a set of components, in which each kind of component has its own criteria and metrics. These collective criteria, applied at the technology-base level, determine whether or not a functional system of a particular kind in consideration can be constructed, even in principle. They are interdependent, because each set of component criteria is meaningful only in the context of some specific range of system-level designs, in which they are criteria for compatibility and completeness.

Condition (3) is based on metrics. Together with (1) and (2), these metrics collectively determine whether or not a technology base is sufficiently advanced that concrete system-development activities have a realistic possibility of producing results of practical value. They, too, are interdependent, because "adequate performance" is meaningful only in the context of some specific range of system-level designs.

Criteria and metrics in developing a technology base in a new area

In developing improved systems of familiar kinds, there is a familiar technology base that already meets conditions (1) and (2). Engineering teams can be led by experienced designers, and they can focus on problems related to new designs and to improvements in area (3). New generations of semiconductor products fit this model.

In the early stages of developing fundamentally novel systems, by contrast, engineering teams and experienced designers do not yet exist, and determining the criteria (1) and (2), and the appropriate performance metrics, is itself a research task, one that requires exploratory engineering to generate coherent candidate system concepts. Many promising areas of atomically precise system design and fabrication are in this exploratory phase. Molecular digital logic systems are one example.

In established areas of research and engineering, basic functional criteria are usually implicit, metrics are well known, and differences among competing products are often small. In new areas, where components of new types have not yet been used in systems, it becomes important to make even the most elementary functional criteria explicit, and to apply what may be unfamiliar metrics.

Further, competing device technologies may be of radically different kinds, and not yet demonstrated. Metrics can still be assessed, within some range of uncertainty, on the basis of descriptive physical models. When assessments reveal multiple-order-of-magnitude differences in potential performance, this may have a significant influence on the allocation of research funds.

Criteria and metrics in reporting and applying research results

Scientific research results are often published in a form that greatly limits the value of the research to engineers. To determine whether a material, a molecule, or a physical phenomenon can be used to solve an engineering problem, the relevant data must have been recorded and reported. By requiring research reports to describe results in terms of the metrics relevant to the intended areas of application, researchers will have an incentive to gather and report data relevant to both exploratory and production-oriented engineering.

The utility of research results can be further increased by indexing the results in a database in a way that facilitates access by engineers who are seeking to generate and test ideas for solving specific problems, or are seeking data to improve the accuracy of their models. Without a standard format for reporting the relevant information, it will be scattered through the text of journal articles written by scientific specialists, and intended to be read by others in the same field. Indexing results by the criteria that describe their nature, and by the values of their relevant metrics, would make research results more accessible, and thereby multiply their value.

For example, an engineer exploring the potential for engineering biomolecules to direct the growth of metal nanorods might want to search for results that report the synthesis of metallic nanoparticles in water at less than 100°C. The relevant papers would meet the simple criteria for describing a 'synthesis', and they would report the quantitative metric 'temperature of synthesis' as 100°C, and the set of 'solvent composition' metrics as 100% for 'water', and the set of 'product composition' metrics would have non-zero values for the appropriate metals.

The value of this way of reporting results suggests that it may be valuable to organize a review of existing papers in selected areas, in which reviewers would index them according to selected metrics that are useful and frequently reported. In the above example, the search would recover papers like these: "Room Temperature, High-Yield Synthesis of Multiple Shapes of Gold Nanoparticles in Aqueous Solution",[81] "Novel one-step synthesis of amine-stabilized aqueous colloidal gold nanoparticles",[82] and "Biomimetic synthesis and patterning of silver nanoparticles".{c83}

Criteria and metrics in managing research

There can be several possible outcomes of assessing whether a research result meets the criteria for filling a role in a system.

- ***Confirms potential value:*** The assessment may determine that a result does, in fact, meet the intended criteria.
- ***Identifies unmet quantitative requirements:*** The assessment may find that a result is of the right kind, but lacks necessary performance, possibly indicating that improvements would be of value in this context
- ***Identifies unmet qualitative requirements***: The assessment may find that a result is of a kind that cannot serve a claimed function, and that improvements would, for the purpose under consideration, have no value.
- ***Reveals unexpected potential value:*** The information used in the assessment may be compared to other criteria, and reveal that the result can serve an unexpected function. Note that this may be discovered at a later date, particularly if criteria and metrics data are used to organize research results to make them useful to engineers searching for solutions to problems in a design.

Metrics can be used to measure improvements, and together with an engineering sensitivity analysis, they can be used to judge the relative value of improvements of different kinds for specific applications. On a larger scale, metrics can provide a transparent and objective basis for incentives and program review. In judging programs, the relevance and effectiveness of research can be assessed in part by whether its research results meet the criteria for relevance to valuable application areas, and whether the associated metrics indicate these research results are advances.

As noted in the introduction, many other considerations enter into assessments of research programs, proposals, and results. These include cost, likelihood of success, the value of diverse approaches, the added value of research that can serve multiple purposes, and the possibility of surprising and useful discoveries. At the level of laboratories, academic research work and achievements, workforce and talent training, openness and academic exchange, and operation and management are established components of assessment.[84]

Application-oriented criteria and metrics are essential for assessments in engineering development, and less important for assessments in basic science. Even in the most basic nanoscience, however, it can be very valuable for results to be reported in terms of relevant engineering criteria and metrics. These provide a common language for comparing physical systems, and they help to organize data in a way that makes it accessible and useful for engineering activities of all kinds.

Case studies of criteria and metrics:

As an example, criteria and metrics are applied to two contrasting research programs in molecular digital logic.

Criteria for qualifying as a digital logic systems technology:

To qualify as a digital logic systems technology (either proposed or implemented), a technology must provide a set of devices that meets the following criteria:

(1) Universal operator set: Logic gates provide a universal operator set (for example, AND, OR, and NOT gates)

(2) Composability: Logic gate output signals can serve as inputs to other logic gates

(3) Controlled connectivity: Logic gate output signals can be directed to specific other logic gates with acceptable signal leakage

(4) Fanout: Logic gate output signals can provide input signals to multiple other logic gates

(5) Signal restoration: The strength of signals either does not decay or can be restored from a low level to a standard level

Criteria for qualifying as a digital logic gate:

To qualify as a digital logic gate (either proposed or implemented), a device must meet the criteria for serving as a logic gate in one or more digital logic systems designs (either proposed or implemented).

Metrics for a digital system logic gate (a partial list):

- Gate delay
- Energy dissipation
- Error rate
- Operating temperature
- Device area
- Leakage current
- Operating voltage

Case study #1: A retrospective application of criteria and metrics to a proposed digital logic gate that was inherently unable to meet the criteria, together with a follow-on discussion of the failure of the 15 years of subsequent research on similar "digital logic".

This example is based on the publication "A molecular photoionic AND gate based on fluorescent signalling", de Silva, Gunaratne, and McCoy, *Nature* **364:**42–44 (1993).[60]

Assessed function: Digital logic gate

Structure and principle of operation:

Input signals are hydrogen ions, sodium ions, or both. Components are organic molecules. Output signal is a change in fluorescence properties.

Criteria:	**Score**	**Reason**
(1) Member of operator set?	✔	the logic operation is "AND"
(2) Composability?	✘	the outputs cannot serve as inputs
(3) Controlled connectivity?	✘	the devices cannot be connected
(4) Fanout?	✘	the devices cannot be connected
(5) Signal-level restoration?	✘	not meaningful

Metrics:

inapplicable

Net assessment:

Fails to meet criteria.

Comments:

No device using chemical signals and fluorescent outputs can serve as a logic gate in any reported digital logic system concept. Further work on molecular devices of this kind can be expected to have no value in digital logic system applications.

The outcome of subsequent research:

Update, 2007: Failure to produce logic systems

Since 1993, active research on devices of this kind (some of it in China) has never connected the output of one "logic device" to the input of another, confirming the formal criteria-based assessment shown above, yet researchers continue to claim to have made contributions to digital computation: "Molecular logic and computing", de Siliva and Uchiyama, Nature Nanotechnology 2:399 - 410 (2007) and "Molecular logic devices (half-subtractor, comparator, complementary output circuit) by controlling photoinduced charge transfer processes", New J. Chem., 32:395–400 (2008).

Update, 2008: Success in producing sensors

Failure to meet criteria in one area does not preclude success in another. For example, de Silva's devices meet the criteria for being sensors, and they are now used in a blood analysis product with over US$50 million annual sales reported in 2008.[85]

Case study #2: A candidate digital logic system that meets the criteria, but forces the definition of new metrics for a new category.

This example is based on the publication "Enzyme-Free Nucleic Acid Logic Circuits", Seelig, Soloveichik, Zhang, and Winfree, Science, 314:1585–1588 (2008).

Assessed function: Digital logic system

Structure and principle of operation:

Input and output signals consist of single-stranded DNA molecules. Each logic gate consists of double-stranded DNA molecules. All signal and gate molecules are present in the same aqueous solution at the same time and in significant concentrations. Binding of a single-stranded signal molecule to a double-stranded gate molecule displaces one or more other single-stranded molecules, freeing these into solution for subsequent interaction with other gates. DNA sequence complementarity makes binding specific, associating each signal molecule with a specific gate.

Criteria:	**Score**	**Reason**
(1) Universal operator set?	✔	includes AND, OR, and NOT
(2) Composability?	✔	outputs can serve as inputs
(3) Controlled connectivity?	✔	specificity of DNA hybridization
(4) Fanout?	✔	demonstrated
(5) Signal -level restoration?	✔	demonstrated

Metrics:

Gate delay	hours
Energy dissipation	not reported
Error rate	potentially negligible
Operating temperature	25°C
Device area	*Not applicable*
Leakage current	*Not applicable*
Operating voltage	*Not applicable*

Net assessment:

Meets stated criteria; inapplicable metrics indicate a need for establishing a new category of digital logic systems, with different metrics.

Comments:

The study reports the development and demonstration of a logic system consisting of 11 gates. Both the design methodology and component production methods are simple.

The identification of inapplicable metrics (area, current, voltage) provides a direct, formal indication that this system must be placed in a separate class from electronic systems, which indicates a need for added criteria and assessment in a new system context. This indicates fundamental novelty.

B5. Identifying objectives:

applications of exploratory engineering

As discussed previously, exploratory engineering develops and analyzes concepts for useful systems before the means for implementing those systems have been developed. Early in research, these concepts may be very general, and the analysis very approximate. Closer to development, exploratory engineering evolves toward more conventional conceptual design, which is constrained more tightly by the capabilities of available or soon-to-be-available technologies, and uses more accurate approximations as a basis for analysis. This, in turn, transitions to product engineering, where the most attractive concepts are refined into detailed, implementable designs, supported by analysis at standard engineering levels of accuracy and precision.

Information products from exploratory engineering

Exploratory engineering can be used to produce several kinds of information products that are necessary for the purposes of defining system-development objectives, related criteria and metrics, and relationships between component and system performance. All of these are important in setting research priorities:

System-level exploratory design: Describe new concepts and alternative implementations and for useful systems in terms of their mode of operation, and the basic characteristics.

- For example, describe alternative surface interfaces, signal paths, and switchable structures in a memory cell in a self-assembled integrated-circuit overlay

System-level exploratory analysis: As part of exploratory design, apply physical and engineering principles to assess and compare alternatives by providing quantitative evaluations of the relationships among their components.

- For example, assess the ability of proposed signals to switch proposed devices, the range of possible switching speeds that might be achieved, and the range of system-level performance properties that might be achieved.

Component criteria: Based on a system-level analysis, describe the basic characteristics of the processes and components that the system requires.

- For example, signal paths in self-assembled systems must transmit signals across the relevant self-assembled interfaces.

Component metrics: Specify the quantifiable properties of components and processes that are important to system design and performance.

- For example, cell volume, switching speed, energy dissipation, and error rate are standard metrics that apply across most digital logic technologies.

Sensitivity analysis: Describe the quantitative relationship between component metrics and system performance.

- Note that this relationship may be weak: For example, although the mass of a component is a common engineering metric, efforts to reduce the mass of a nanoscale transistor would have no perceptible value.

These information products provide information necessary to structure a successful system-development research program.

Applications of information from exploratory engineering

Defining system-level research objectives: Given the goal of developing a technology that serves a particular need, exploratory system-level design and analysis provide a means to identify and compare alternative implementations of systems that can satisfy the requirements. A formal exploratory engineering process increases the likelihood of identifying approaches that are better in terms of cost, development risk, and product performance. An informal process increases the likelihood that researchers will pursue poorly defined goals that have never been carefully examined.

Identifying a complete set of component-level research objectives: Given the goal of implementing a system of a particular kind, it is necessary to have or develop all of the necessary components. A formal system-level description and analysis ensures that these are explicitly listed so that none will be omitted. An informal process increases the likelihood that a development program will be delayed, or fail, because some necessary components or processes are unavailable, and increases the likelihood that resources will be wasted on developments that appear to be relevant, but in fact are unnecessary.

Assessing research programs, proposals, and results: As discussed in Sections B4 ad B5, criteria, metrics, and sensitivity analysis can provide transparent and objective ways to assess research programs, proposals, and results. In the context of new technologies, performing exploratory design and analysis provides a way to identify requirements, and from these, to define formal criteria and metrics, and to assess the relative value of improvements in different metrics. An informal process, by contrast, is likely to neglect necessary criteria in assessing the relevance of research, and is unlikely to give proper weight to the metrics that determine the practical value of a result.

Table B5: A comparison of production-oriented and exploratory engineering.

	Production-oriented engineering	**Exploratory engineering**
Objective	Create and evaluate system-level designs (typically parameterized)	— *Same* —
Background technology	Known capabilities of current fabrication technologies	Conservative, physics-based estimates of the capabilities of future fabrication technologies
Process of analysis	Identify required subsystems and components, and their required performance parameters	— *Same* —
Basis of calculations	Typical performance of available materials and components (Design may exploit poorly understood phenomena)	Conservative, physics-based estimates of lower bounds on the performance of feasible materials and components. (Design must avoid poorly understood phenomena)
Results of calculations	Estimates of the performance of fully refined, system-level designs	Lower-bound estimates of the performance of fully refined, system-level designs
Production and performance	Product must be manufacturable and competitive today	Product is not manufacturable today, and need not be competitive in the future
Implication for design criteria	Seek efficient configurations to maximize performance and minimize cost of production	Seek simple designs and assume large design margins to maximize confidence and minimize cost of design analysis
Results of the design process	Choice of system-level design concepts for refinement and possible production	Estimates of the capabilities of future levels of fabrication technology for evaluation of research and policy options

Exploratory engineering can help guide research and development

A spectrum of levels of engineering

Setting objectives for an application-oriented research program requires the exploration and analysis of design concepts at an appropriate level of specificity and detail. In advanced stages of development, it is appropriate to apply a conventional, detailed, production-oriented engineering approach. At the earliest stages of research, however, it is more appropriate to survey a range of design concepts, in order to catalog their general requirements and to identify the physical metrics that determine the performance of components, systems, fabrication processes, and so forth. Even at the basic science stage of research, it is important to report physical parameters of engineering interest, as an aid to assessing whether the results point to possible applications.

These design-oriented activities form a continuum. Conventional engineering typically designs systems that resemble previous systems: Materials and components are typically similar or identical to those already in use, and the organization of the system is usually of a familiar kind, or nearly so. Because of this, the metrics are usually familiar, and the relevant criteria may be too obvious to mention. In engineering a digital logic system, for example, the metrics of gate delay, power dissipation, and so on, are familiar, and the criteria for a device to be an 'AND gate' need not be discussed.

In exploratory engineering for nanotechnology, by contrast, the crucial roles of new phenomena, new devices, and new kinds of systems all increase the difficulties of assessing research objectives, proposals, and results. Methods for judgment in this domain often require more explicit attention to fundamental questions that can be answered by exploratory engineering design and analysis, and the application of the resulting criteria and metrics.

The appropriate level of specificity for design concepts varies with the stage of research. Both general and specific design concepts indicate the need for criteria and metrics for nanowires, for example, but more specific design concepts are necessary to determine criteria and metrics for quantum wires that self-assemble with quantum dots to form photochemically stable assemblies for high-efficiency solar photovoltaics.

As a set of capabilities matures, exploratory engineering transitions smoothly to the generation of alternative design concepts for implementation. This process ultimately leads to the refinement of detailed designs for functional products and of processes for their manufacture. Explicit exploratory engineering can produce system-level descriptions of products and their requirements as an aid to directing and evaluating application-oriented research.

Exploratory engineering both generates and uses criteria and metrics

There is a bi-directional relationship between exploratory engineering and research assessment based on criteria and metrics. In one direction, exploratory engineering plays a central role in determining appropriate criteria and metrics for research. In the other direction, systematic assessment of research based on criteria and metrics will by nature produce data of the kind necessary for engineering analysis.

Criteria and metrics are intimately related to engineering analysis. Criteria and metrics define the properties of the components that are the building blocks of engineering analysis, and in new areas, it is engineering analysis that defines the roles of new components, and in defining those roles, it requires the definition of the corresponding criteria and metrics. In areas of research that discover new materials, phenomena, and structures, the process of describing and analyzing their potential applications directs attention to the questions that must be answered, and to the requirements that must be met by further development.

Exploratory engineering can break barriers to progress

Without exploratory engineering and analysis, it may be impossible to know whether a field is or is not ready to advance toward applications. By exploring alternatives and their requirements, exploratory engineering may uncover shorter paths than those that had been assumed. This can be of enormous importance, because assuming that a capability is a requirement, when it is in fact unnecessary, can delay progress indefinitely. The process of considering a technology from a design-oriented, problem-solving perspective challenges these assumptions and can therefore break down conceptual barriers to proceeding more directly to implementation.

For example, in the field of protein engineering, scientists had assumed that it would be necessary to understand and predict how natural proteins fold before engineering artificial proteins would be possible. Examining the problem from an engineering perspective showed that this would be unnecessary.[14] this opened the door to developing practical methodologies for protein engineering[86] at a time when the natural-protein fold prediction problem was far from being solved.

Conservative exploratory engineering can be applied to HT-APM

Product performance: Conservative exploratory engineering enables lower-bound projections of the performance of a range of HT-APM products.

The concept of HT-APM relies on exploratory engineering conducted according to a methodology that enables a high confidence in lower-bound estimates of performance. This methodology, as applied to HT-APM, is discussed in more detail in Section B5.

As a rule, confidence in an engineering analysis can be increased by applying conservative assumptions and wide error margins to simple designs, and this principle can be applied to designs that are far from standard engineering practice.

For products of HT-APM technology, designs that are chosen for ease of analysis—and are far from optimal in a conventional engineering sense—can yield highly conservative lower-bound performance metrics that exceed those of current well-engineered products by a large factor. High performance, by present standards, is often compatible with extremely conservative engineering, provided that the analysis is applied to a technology base that can fabricate large objects from a wide range of materials with atomic precision.

Process performance: Conservative exploratory engineering enables lower-bound projections of the performance of a range of HT-APM processes.

Atomically precise structures and processes, based on organizing the fundamental building blocks of matter, have a wide range of unique engineering properties. One of those properties is that a conservative exploratory engineering analysis can be applied to the production process itself, and result in a lower bound on performance that is, by current standards, extraordinarily high.

At the molecular level, where reactive molecular building blocks are combined to make materials and nanoscale devices, fabrication based on mechanical constraint of encounters between reactive molecules is a very powerful technique. Because production machinery of this sort can be used to make a range of products including production machinery of the same kind, the analysis permits a unique degree of closure with respect to materials flow, energy consumption, and production of capital equipment. The physical principles that underlie this analysis are outlined in Section B3. All of them are familiar to engineers and physicists, and are readily comprehended by undergraduate students in these fields.

Exploratory engineering in the domain of HT-APM has shown that, with a set of highly conservative assumptions throughout the analysis, the metrics for production throughput and product quality and performance far exceed those of production processes in use today. The physical differences between HT-APM and current production systems are profound, the quantitative difference in performance is correspondingly large, and the potential results of the resulting capabilities are enormous, in a literal, physical sense.

SIDEBAR B7

What is the purpose of a technology roadmap?

Below are the self-described purposes of technology roadmaps in areas that range from the industrial concerns of water desalination to the scientific frontiers of quantum computing. These descriptions share the central theme of improving the coordination of research and development, and they offer several perspectives on the problems and how roadmapping helps to resolve them.

Desalination and Water Purification Technology Roadmap

"Technology roadmaps serve as pathways to the future. They call attention to future needs for developments in technology, provide a structure for organizing technology forecasts and programs, and communicate technological needs and expectations among end users and the research and development (R&D) community."

Source: *Desalination and Water Purification Technology Roadmap* (2003). U.S. Department of Interior, Bureau of Reclamation: http://www.usbr.gov/pmts/water/media/pdfs/report095.pdf

The International Technology Roadmap for Semiconductors

"...it is the purpose of the ITRS documents to provide a reference of requirements, potential solutions, and their timing for the semiconductor industry. This objective has been accomplished by providing a forum for international discussion, cooperation, and agreement among the leading semiconductor manufacturers and the leading suppliers of equipment, materials, and software, as well as researchers from university, consortia, and government labs.

"The ITRS documents have become and remain a truly common reference for the entire semiconductor industry. Indeed, the cooperative efforts of the ITRS participants have fostered cooperation among international consortia, universities, and research institutions around the world."

Source: *The International Technology Roadmap for Semiconductors* (2006 Update). Overview and Working Group Summaries: http://www.itrs.net/Links/2006Update/FinalToPost/00_ExecSum2006Update.pdf

Quantum Information Science and Technology Roadmap

"The roadmap is intended to function in several ways to aid this development. It has a prescriptive role by identifying what scientific, technology, skills, organizational, investment, and infrastructure developments will be necessary to achieve the desired goal, while providing options for how to get there. It also performs a descriptive function by capturing the status and likely progress of the field while elucidating the role that each aspect of the field is expected to play toward achieving the desired goal. The roadmap can identify gaps and opportunities, and places where strategic investments would be beneficial. It will provide a framework for coordinating research activities and a venue for experts to provide advice. The roadmap will therefore allow informed decisions about future directions to be made, while tracking progress, and elucidating interrelationships between approaches to assist researchers to develop synergistic solutions to obstacles within any one approach. The roadmap is intended to be an aid to researchers and to those managing or observing the field."

Source: *A Quantum Information Science and Technology Roadmap (Verson 2.0), Report of the Quantum Information Science and Technology Experts of the U.S. Advanced Research and Development Activity (ARDA)* (2004): http://qist.lanl.gov/pdfs/rm_intro.pdf

continued...

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Criteria and metrics in the three technology roadmaps

Criteria and metrics permeate the subject matter of technology roadmapping, and technology roadmap documents, and metrics are often stated explicitly.

Desalination and Water Purification Technology Roadmap

Metrics are used to define critical objectives:

"It is expected that institutions funding or conducting desalination and water purification research will use this Roadmap to make decisions about research direction and use the Roadmap's metrics to document progress toward meeting the identified Critical Objectives and embrace the Vision for desalination and water purification technologies."

The International Technology Roadmap for Semiconductors

Metrics and associated timelines are used by companies to estimate the targets they must meet to be competitive:

"The Overall Roadmap Technology Characteristics (ORTC) tables are created early in the Roadmap process and are used as the basis for initiating the activities of the International Technology Working Groups in producing their detailed chapters."

The ORTC metrics are often used by semiconductor companies as a set of targets that need to be achieved ahead of schedule to secure industry leadership."

Quantum Information Science and Technology Roadmap

In quantum computing, as in nanosystems technologies, criteria for functional systems must be explicit. The quantum technology roadmap therefore includes the ' DiVincenzo criteria':

"...the roadmap presents a 'mid-level view' that segments the field into the different scientific approaches and provides a simple graphical representation using a common set of criteria and metrics to capture the promise and characterize progress towards the high-level goals within each approach."

"To represent the promise of each approach [to quantum computing] the panel decided to adopt the 'DiVincenzo criteria.'"

The DiVincenzo criteria state a set of necessary conditions for any viable QC technology: It must provide a scalable set of quantum bits with states that can be initialized, maintained, transformed by gates, and read.

B6. Technology characteristics and national security risk management

Section 5.3 outlined aspects of the military potential of technologies at the level of HT-APM, and discussed reasons why adversarial development of this level of technology would create large and unnecessary risks of military surprise. The consequences of these risks extend in magnitude from rapid obsolescence of weapons and strategic doctrines to threats to continued existence at a national level.

This suggests that adversarial development would be a high-risk strategy. Further, the technology itself will, by nature, change objective facts that are critical to the national interest of great powers in the 21st century. In particular the same fundamental technology will greatly reduce requirements for scarce raw materials, and will thereby reduce a large and growing source of international tension.

In considering these developments, it is natural to think in terms of analogies to previous technological advances of first-rank military significance. Nuclear weapons provide a reference point, and it is important to examine the analogy carefully, because the differences are greater than the similarities. Contrasts include:

- Potential pace of development and deployment and the ability to monitor it
- Range of applications and predictability of their military consequences
- Contributions to problems of health care, global environment, and development
- The role of cooperation both in reducing risks and in creating value for society

Table B6 summarizes similarities and differences in greater detail.

Table B6: Comparison of advanced nanotechnologies and nuclear weapons technologies. A comparison between nuclear explosive devices and HT-APM-based technologies from the perspectives of development paths, military applications, arms control, and peaceful applications shows large contrasts.

Aspect of technology	Nuclear explosive devices	HT-APM systems and products
Military importance	Crucial strategic importance	Crucial strategic importance
Development paths	Well explored	New and potentially surprising
Necessary facilities	Large, specialized	Laboratory scale, common
Critical enabling tools	Physical tools for production	Software tools for design
Critical enabling resource	Special nuclear materials	Special design information
Information leaks	Cannot transfer physical tools and materials	Can transfer software tools and design information

Military effects	Devices destroy large targets, contaminate wide areas	Potential products include diverse systems with diverse effects
Military applications	Since 1950, primarily strategic deterrence	Potential applications in defense, offense, and cooperative security
Assessment of forces	Can estimate force capabilities, and changes are slow	Both the nature and magnitude of capabilities may be unknown, and changes can be rapid
Risk of major surprises	History records repeated surprise developments	Equal or greater potential for surprise developments
Motive for preemption	Anticipated technology development has motivated preemptive military strikes	Potentially similar motivations based on worst-case analyses of unknown threats
Deterrence of use	Deterrence relies on nuclear weapon use being a unique, recognizable, hostile action	Potential products have pervasive applications in both civil and military activities of all kinds
Definability in negotiations	A unique class of devices with special enabling technologies and few applications	Extraordinarily diverse products with generic enabling technologies and pervasive applications
Monitoring of agreements	Can require on-site inspection of nuclear-technology sites	Would require extensive transparency across multiple areas of research
Cooperative development	Cooperative development has facilitated widespread peaceful use of nuclear energy.	Deep, broad, transparent cooperation could accelerate development of peaceful and stabilizing applications, and could provide the extensive transparency necessary to implement agreements that can reduce military and other risks
Environmental applications	Few or none	Reduce resource requirements, eliminate toxic emissions, transition to a zero-net-carbon economy
Medical applications	Radioisotope production (can be separated from weapons production)	New, curative treatments for cancers, new and drug-resistant pathogens, and many chronic conditions
Economic applications	Energy production (can be separated from weapons production)	Accelerated and sustainable global development, greatly reduced competition for scarce energy and material resources

B7. Integrating research:

applications of technology roadmapping

Ongoing roadmap development is an institutional process by which specialists in diverse areas of science and technology (at stages of development ranging from scientific exploration to industrial production) can learn about one another's capabilities and can formulate a better understanding of how these can be advanced and combined. The process of roadmap development can advance exploratory engineering concepts to the level of concrete plans for developing the necessary components and integrating them to form working systems. It can refine and build consensus on criteria and metrics that can guide both competitive development of alternative technologies and cooperative development of complementary technologies.

Table B7: A scorecard for institutional openness and collaboration

Implementation of policies for openness and collaboration:	
Researchers participate in technology roadmap development	✔
Researchers participate in developing design-oriented criteria and metrics	✔
Research results are indexed by criteria and metrics in an open database	✔
Incentives are aligned with standard criteria and metrics for progress	✔
Businesses fund or collaborate in applied research	✔
Laboratories are open to visiting researchers	✔
Researchers participate in external collaborations	✔
Researchers participate in international collaborations	✔
Provide specialized user facilities [1] for external researchers	✔
User facilities are available on an international basis	✔
Provide specialized service facilities [2] for external researchers	✔
Service facilities are available on an international basis	✔

(1) A *user facility* enables visiting researchers to use special equipment with the help of technical personnel

(2) A *service facility* provides specialized services (for example, chemical synthesis, computational modeling, chemical analysis, electron microscopy) in response to requests

The first section of Sidebar B7 offers descriptions of the purpose of technology roadmapping, quoted from several roadmaps developed in fields of research and industrial development. The second section shows how those roadmaps and their users apply metrics and, where necessary, explicitly articulated criteria. Section B4 discusses the role of criteria and metrics in nanosystems development, and offers case studies of their application to research in molecular digital logic systems.

It is important to keep in mind that technology roadmapping serves two complementary and fundamentally different functions: Discovery processes that broaden options and reveal strategic alternatives, and planning processes that narrow options and produce concrete decisions. In this, a technology roadmap is like a literal map of roads. A roadmap can provide an overview of a region, revealing alternative destinations, and once an attractive destination has been chosen, a roadmap can help a planner to judge distances and select the most direct path.

Technology roadmapping and technology-base roadmapping

Experience shows that the technology base for any class of complex, heterogeneous systems will consist of many complementary technologies, because the systems themselves will contain many kinds of materials and components, and will therefore require complete suites of compatible technologies for design and fabrication. This is seen both in factory systems and their products. Even a century ago, automobile production required many materials (copper, glass, rubber, and many kinds of steel) in the form of components ranging from wires to sheet metal to engine blocks. Since then, the automotive technology base has expanded to include robotics for manufacturing and nanoelectronics for on-board computation.

In fields undergoing incremental progress, an informal, implicit sort of technology roadmapping takes place even without explicit formal organization. Suppliers and customers have ongoing relationships through which expected, incremental advances and requirements can be discussed. Today, explicit business-level technology roadmapping is increasingly being formalized and extended, to the point of supporting development of specialized software for supporting technology roadmapping in business[87] and academic studies of the optimization of roadmapping processes for different business needs.[88] This kind of technology roadmapping, however, is focused on business strategic planning in an environment of incremental technological advance and the occasional emergence of new product categories and industry-wide transformations.

The kind of technology roadmapping required in nanotechnology development today overlaps with incremental roadmapping, but centers more heavily on non-incremental change in the form of the emergence of new device principles, new materials, new fabrication technologies, and new kinds of nanosystems. This might better be termed ‘technology-base roadmapping’, because it operates at a broader and deeper level of change. The roadmaps cited in Sidebar B7 are toward the technology-base end of the roadmapping spectrum. The quantum information technology roadmap occupies the position furthest in this direction. The most outstanding example of an ongoing technology-base roadmapping effort, the International Technology Roadmap for Semiconductors (ITRS),[63] is in the middle of this spectrum.

It is important to recognize that a coherent technology base for nanosystems is unlikely to be produced by a thousand laboratory groups working independently, no matter how brilliant the researchers may be, or what scientific breakthroughs they may achieve. Independent or loosely coordinated groups are likely to pursue tasks of intrinsic interest, with no specific mechanism for recognizing and prioritizing problems that must be solved in order to build systems. In areas of technology base development far enough advanced to enable system development, the need is even more acute: Concrete products require components that fit together in a literal sense—standardized sizes, shapes, interfaces, as well as more abstract forms of ‘fit’, such as compatible process and operating conditions.

Technology-base roadmapping spans a range of levels. It focuses work on seeking sets of components that meet fundamental criteria for serving system-level functions (like the 'DiVincenzo criteria' at the center of the quantum information technology roadmap). It orients and motivates competition to meet performance requirements specified in terms of metrics. The result is to drive development of fully compatible sets of physical and design technologies suitable for building complex functional systems.

Technology-base roadmapping establishes a focus of attention on the concept of a technology base, on the system-level development objectives for the technology base, as currently understood, and on the criteria and metrics that establish standards for judging progress in advancing the technology base.

Technology roadmapping and potential roadblocks to system-level innovation

Ultimately, the potential payoff for research and development is the production of valuable functional systems: Computers, instruments, production processes, and so on. Where production of valuable functional systems will require several separate groups to develop mutually complementary technologies, the mutual expectations among those groups are of critical importance. These expectations can foster rapid progress, or they can stabilize a condition of prolonged inaction with enormous opportunity costs.

If the payoff for research and development comes from building valuable systems, then (with appropriate institutions) a research group will be rewarded for developing a technology that enables those systems to be built. However, if the development of a high-value system requires the development of multiple, complementary technologies, the expected payoff for successful results by any one research group may be enormous or negligible, depending on the context. Consider the viewpoint and expectations of a research group that can provide one of the requirements for the valuable system. Any one of the following conditions can result in the research group deciding to pursue other objectives instead, regardless of the magnitude of the potential value of successful development of the system.

Potential barriers to system-level innovation:

1) Exploratory engineering has been inadequate, and so the system concept does not yet exist.

2) The concept exists, but institutionally credible assessment processes have not yet been applied, and so it is not yet a credible objective for development.

3) A credible, high-payoff system-development objective has been defined, but it has not been communicated, so the researchers do not know whether or not they can provide a requirement in their area, and it may not be known whether all the requirements can be satisfied.

4) The researchers know that they can satisfy one requirement for achieving the objective, but some of the other requirements cannot be satisfied, and so the payoff from their contribution would be low.

5) Other groups have the means for satisfying all the other requirements, but the researchers do not know that these means exist, and so they expect that the payoff from their contribution would be low.

6) The research group knows that the other requirements can be satisfied, but they do not expect the other groups to undertake the necessary research, so they expect that the payoff from their contribution would be low, and they do not undertake their part of the necessary research. The others reach the same decision, they prove one another to have been correct, and the opportunity is lost.

In problems (5) and (6), a problem is ready to be solved, but mutual negative expectations make this impossible. This problem is especially likely when the groups with parts of the solution have never before worked together, and this, in turn, is very likely when the opportunity being lost is a transformative breakthrough. Roadmapping can bring together the groups that need to communicate, and can produce a document that creates the necessary mutual positive expectations across the range of fields that must coordinate their actions to provide the requirements for success. Research managers can draw on this document to identify critical requirements that are being neglected, and provide the resources necessary to satisfy them and thereby achieve the high-value objective.

In problem (4), there is a genuine obstacle to success, because there is no known way to solve a critical problem. A roadmapping process can identify this problem as an obstacle that blocks progress toward a valuable objective, and researchers and research managers may judge that it is worth allocating resources to attempt to find what can be recognized as a valuable solution.

In problem (3), it is not yet known whether all the requirements can be satisfied, because the relevant research groups have not had a reason to examine the question. A roadmapping process can bring system concepts to the attention of research groups that may be able to satisfy some of the requirements, and give them an incentive to propose projects that would accomplish this.

Problem (2) can result from a failure to designate experts to assess a concept and report on their conclusions. (For example, the U.S. Federal government took no formal steps to assess the concept and the already-existing analysis of HT-APM until a 2005 study released as part of a general review of the U.S. National Nanotechnology Initiative[79].) Assessment may be difficult because it will typically require the integration of expert knowledge from multiple fields, and specialists in any one field may be unaware of the problems that have already been solved in other fields. Roadmapping processes can address one aspect of this problem by bringing diverse experts together for the purpose of considering problems of system implementation and how they might be solved.

By their nature, roadmapping processes bring together researches from multiple disciplines to discuss how their research results could be combined for practical applications. In contrast to scientific meetings, which foster exchanges among specialists engaged in similar research, roadmapping meetings foster exchanges among specialists with very different and potentially complementary areas of knowledge and capability. These discussions can spark new thinking in many directions, including ideas that, when explored and analyzed, result in concepts for new and potentially valuable systems. In this way, roadmapping can encourage the exploratory engineering processes that address problem (1).

In short, roadmapping processes can create conditions and interactions that foster the emergence and evaluation of innovative system-level concepts, can provide researchers with an opportunity to identify how they can solve new system-enabling problems, identify and focus resources on finding solutions to critical problems, ensuring that all requirements are satisfied, and can induce the cross-disciplinary sharing of information and development of mutual expectations that are necessary for all participants to have confidence that their contributions will, in fact, contribute to producing a high-value system-level result.

Cooperation based on technology roadmapping is used on an industry-wide and international scale

The highly successful *International Technology Roadmap for Semiconductors* states that

> "...the cooperative efforts of the ITRS participants have fostered cooperation among international consortia, universities, and research institutions around the world."
>
> (From: *The International Technology Roadmap for Semiconductors, 2006 Update*, Overview and Working Group Summaries. http://www.itrs.net/Links/2006Update/FinalToPost/00_ExecSum2006Update.pdf)

Technology roadmapping is a form of cooperation, enabling groups to coordinate their activities on an informal basis for mutual benefit at a level that does not require negotiation of payments, facilities sharing, division of intellectual property, or the obligations established by a technology contract.[89] It can help managers spur productive competition by exposing research groups to their potential competitors.

In technology roadmapping, groups in complementary areas have a strong incentive to share information with one another, because together, they may be able to achieve more valuable and rewarding results. Groups competing within a single area have a strong incentive to participate, in order to avoid being left out of new collaborations and left behind in the emergence of new fields of science and technology. These incentives apply within institutions, across industries, and on an international scale.

Technology roadmapping can increase efficiency and reduce risk by fostering division of labor and ensuring that critical work is performed. It can help experts to develop metrics that enable managers to judge proposals and results. In favorable instances, where development requirements are well understood, metrics can be combined with timelines to indicate the performance objectives that must be met for research and development to be competitive, and can indicate the component performance that system designers can expect to be delivered in time for the production of competitive next-generation products.

Evaluating research:
Openness, transparency, control, and decentralization

As discussed elsewhere, a potential response to the special challenges of developing a discipline of AP nanosystems engineering is to expand the use of physical criteria and metrics as a basis for assessing research proposals and research results.

Counting papers vs. measuring progress

There has been a growing emphasis on transparency and openness in S&T administration in China, and this has encouraged the use of objective metrics such as the number of publications (by individuals, groups, and institutions) in journals covered by the Science Citation Index (Sidebar 8).[90] A useful supplement, however, would be objective criteria and metrics that can link the evaluation of results more directly and quantitatively to the needs of technology development, and that can thereby help to shape the direction of supporting S&T. The use of physical criteria and metrics to evaluate research results is one approach to achieving this, and has the additional benefit of being applicable to the evaluation of suitably formulated research proposals.

Necessary complexity

Criteria and metrics of this kind cannot be as simple and extensively applicable as the metric “number of papers” that satisfy the criterion “published in an SCI journal”; however, a greater degree of complexity is a necessary aspect of their utility as a means of focusing research on complex and diverse technology development targets. A further difficulty is that, to be effective for this purpose, criteria and metrics must reflect an evolving understanding of the nature of potential technologies, their value as targets, and the requirements for their implementation. As a consequence, the set of recognized criteria and metrics will expand over time, and the estimated value of satisfying particular criteria and improving particular metrics will inevitably require adjustment.

Transparent development of criteria and metrics

Some fundamental aspects of the development and revision of physical criteria and metrics can be fully open, transparent, and objective. This includes development and revision based on the identification and evaluation of new, high-payoff application concepts through exploratory engineering design and analysis (Background section B5).

Transparency and open evaluation will of course tend to improve the quality of designs and of analysis, sometimes leading to the invalidation, revision, or improvement of an exploratory design concept, or leading to adjustment of the bounds of (potentially very broad) confidence intervals. Information from later research, perhaps in unexpected areas, may also lead to revision.

Some other aspects of the development and revision process will require judgments that are less quantitative, such as the likelihood that a development path will lead to a competitive result, or the likelihood that a new technique will contribute to a development path. The process of developing these judgments is, however, centered on engineering considerations, and can be open and transparent.

An aid in developing and implementing research priorities

Criteria and the valuation of metrics are, in essence, a way to represent research priorities. If used as a significant component of the evaluation of proposals and results, they would create powerful, flexible incentives for researchers, and a basis for competition among groups and institutions. Changes developed through an open, web-based process could make revision of research priorities more responsive to research results, increasing efficiency and decreasing the opportunity costs incurred by the delayed recognition of opportunities. The effectiveness of this process of evaluation and response can be of great importance: History shows that new concepts can motivate changes on all scales of S&T, reaching to the level of creating or redirecting entire fields of research. A more direct link between knowledge and incentives can be expected to lead to faster and better targeted responses to new opportunities.

This approach appears to have merit as a mechanism that can combine efficiency, flexibility, openness, and transparency. In addition, to provide for state needs not satisfied by market mechanisms, this approach can provide a way to advance China's objective of developing systems of S&T administration that combine strong guidance from the center with strong decentralization of particular decisions and control.

Notes and references

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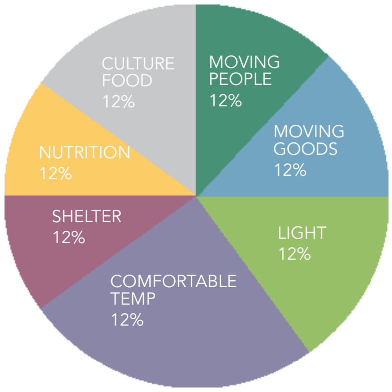

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