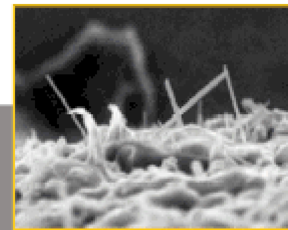
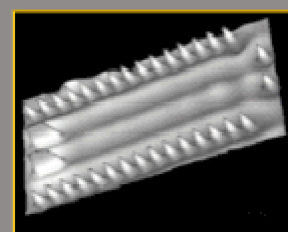
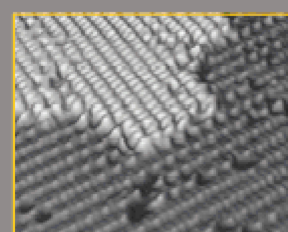
2007

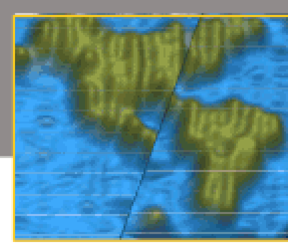
Productive Nanosystems

A Technology Roadmap









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Roadmap Participants

Steering Committee

Paul Alivisatos, University of California at Berkeley
Pearl Chin, Foresight Nanotech Institute
K. Eric Drexler, Nanorex
Mauro Ferrari, University of Texas–Houston, Institute of Molecular Medicine
Doon Gibbs, Brookhaven National Laboratory
William Goddard III, Beckman Institute, California Institute of Technology
William Haseltine, William A. Haseltine Foundation for Medical Sciences and the Arts
Steve Jurvetson, Draper Fisher Jurvetson
Alex Kawczak, Battelle Memorial Institute
Charles Lieber, Harvard University
Christine Peterson, Foresight Nanotech Institute
John Randall, Zyvex Labs
James Roberto, Oak Ridge National Laboratory
Nadrian Seeman, New York University
Rick Snyder, Ardesta
J. Fraser Stoddart, University of California at Los Angeles
Ted Waitt, Waitt Family Foundation

Technical Leadership Team

K. Eric Drexler, Nanorex; Alex Kawczak, Battelle Memorial Institute; John Randall, Zyvex Labs

Project Management Team

Alex Kawczak, Battelle Memorial Institute; K. Eric Drexler, Nanorex; John Randall, Zyvex Labs; Pearl Chin, Foresight Nanotech Institute; Jim Von Ehr, Zyvex Labs

Editors

K. Eric Drexler, Nanorex; John Randall, Zyvex Labs; Stephanie Corchnoy, Synchrona; Alex Kawczak, Battelle Memorial Institute; Michael L. Steve, Battelle Memorial Institute

Contributing Editors

Jeffrey Soreff, IBM; Damian G. Allis, Syracuse University; Jim Von Ehr, Zyvex Labs

Front Cover Design

Katharine Green, Zyvex Labs

Workshop and Working Group Participants

Radoslav R. Adzic*, Brookhaven National Laboratory
Damian G. Allis*, Syracuse University
Ingemar André, University of Washington
Tom Autrey*, Pacific Northwest National Laboratory
Don Baer*, Pacific Northwest National Laboratory
Sandra Bishnoi*, Illinois Institute of Technology
Brett Bosley, Oak Ridge National Laboratory
Joe Bozell, University of Tennessee
Philip Britt, Oak Ridge National Laboratory
Paul Burrows*, Pacific Northwest National Laboratory
David Cardamone*, Simon Frazer University
Ashok Choudhury, Oak Ridge National Laboratory
Stephanie Corchnoy*, Synchrona
James Davenport*, Brookhaven National Laboratory
Robert J. Davis*, The Ohio State University
Shawn Decker, South Dakota School of Mines
Mitch Doktycz*, Oak Ridge National Laboratory
Eric Drexler*, Nanorex
Joel D. Elhard*, Battelle Memorial Institute
Jillian Elliot, Foresight Nanotech Institute
Doug English*, University of Maryland
Leo S. Fifield*, Pacific Northwest National Laboratory
Keith Firman*, University of Portsmouth
David Forrest*, Institute for Molecular Manufacturing; Naval Surface Warfare Center
Robert A. Freitas Jr.*, Institute for Molecular Manufacturing
Glen E. Fryxell*, Pacific Northwest National Laboratory
Dan Gaspar*, Pacific Northwest National Laboratory
David Geohegan*, Oak Ridge National Laboratory
Anita Goel, Nanobiosym
J. Storrs Hall*, Engineering Research Institute, Institute for Molecular Manufacturing
Alex Harris, Brookhaven National Laboratory
Amy Heintz*, Battelle Memorial Institute
Evelyn Hirt, Pacific Northwest National Laboratory
Linda Horton, Oak Ridge National Laboratory
Ed Hunter*, Sun Microsystems
Ilia Ivanov*, Oak Ridge National Laboratory
Neil Jacobstein*, Institute for Molecular Manufacturing
Evan Jones, Pacific Northwest National Laboratory
Richard Jones, University of Sheffield

* Provided material for inclusion in this Nanotechnology Roadmap.

Workshop and Working Group Participants, Continued

John Karanicolas*, University of Washington
Alex Kawczak*, Battelle Memorial Institute
David Keenan, Nanoscience Technologies
Peter C. Kong*, Idaho National Laboratory
James Lewis*, Foresight Nanotech Institute
Alan Liby, Oak Ridge National Laboratory
Khiang Wee Lim, Singapore Engineering Research Council
Eric Lund, Pacific Northwest National Laboratory
Russ Miller, Oak Ridge National Laboratory
Jim Misewich, Brookhaven National Laboratory
Scott Mize, Foresight Nanotech Institute
Lorrie-Ann Neiger, Brookhaven National Laboratory
Lee Oesterling*, Battelle Memorial Institute
Lori Peurrung, Pacific Northwest National Laboratory
Casey Porto, Oak Ridge National Laboratory
John Randall*, Zyvex Labs
Fernando Reboredo*, Oak Ridge National Laboratory
Mark Reeves, Oak Ridge National Laboratory
Steven M. Risser*, Battelle Memorial Institute
Sharon Robinson*, Oak Ridge National Laboratory
Paul W. K. Rothemund*, California Institute of Technology
Jay Sayre*, Battelle Memorial Institute
Christian E. Schafmeister*, Temple University
Thomas Schulthess, Oak Ridge National Laboratory
Nadrian Seeman*, New York University
Ida Shum, Idaho National Laboratory
Mark Simpson, Oak Ridge National Laboratory
Dennis Smith*, Clemson University
Vincent Soh, Singapore Engineering Research Council
Jeff Soreff*, IBM
Rob Tow, Sun Microsystems
Mike Thompson, Pacific Northwest National Laboratory
Bhima Vijayendran, Battelle Memorial Institute
Chiming Wei*, American Academy of Nanomedicine
Chia-Woan Wong, Singapore Engineering Research Council
Stan Wong*, Brookhaven National Laboratory

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Notice

Executive Summary

Atomically precise technologies (APT) hold the potential to meet many of the greatest global challenges, bringing revolutions in science, medicine, energy, and industry. This technology roadmap points the way for strategic research initiatives to deliver on this promise.

APT — An Essential Research Frontier

The long-term vision of all nanotechnologists has been the fabrication of a wider range of materials and products with atomic precision. However, experts in the field have had strong differences of opinion on how rapidly this will occur. It is uncontroversial that expanding the scope of atomic precision will dramatically improve high-performance technologies of all kinds, from medicine, sensors, and displays to materials and solar power. Holding to Moore's law demands it, probably in the next 15 years or less.

Atomically precise technologies are here today in diverse but restricted forms: APT structures are found throughout materials science, and APT products are common in organic synthesis, scanning probe manipulation, and biomolecular engineering. The challenge is to build on these achievements and expand them to produce a wider range of structures, providing APT systems of larger scale, greater complexity, better materials, and increasingly higher performance. Progress in this area can be used to make advances in the area of APT fabrication, which can be used to make further progress in other areas. Physics-based modeling indicates that this path will lead to the emergence of revolutionary capabilities in atomically precise manufacturing (APM).

Reasons why atomically precise manufacturing (APM) and atomically precise productive nanosystems (APPNs) merit high priority:

- *Atomic precision is the guiding vision for nanotechnology.*
- *Limited atomically precise fabrication capabilities exist today.*
- *Prototype scanning-probe based APM systems exist in the laboratory and demonstrate AP operations on semiconductor systems.*
- *Nanoscale APPNs exist in nature and fabricate uniquely complex AP nanostructures in enormous quantities.*
- *Improved AP technologies will enable development of next-generation APM systems.*
- *Next-generation APM systems will enable development of more advanced AP technologies.*

APM Will Launch an Industrial Revolution

Atomically precise manufacturing processes use a controlled sequence of operations to build structures with atomic precision. Scanning probe devices achieve this on crystal surfaces. Biomolecular machines achieve this in living systems. In both technology and nature, the components of complex atomically precise systems are made using APM processes.

Recently identified approaches for using products of today's APM to organize and exploit other functional nanoscale components show great promise. Building on achievements in other areas of nanotechnology, they point to capabilities that could prove transformative in multiple fields, expanding the set of nanoscale building blocks and architectures for products.

Reasons why atomically precise manufacturing (APM) and atomically precise productive nanosystems (APPNs) merit high priority (continued):

- *Nanosystems in nature demonstrate that APPNs can produce solar arrays, fuels, complex molecules, and other products on a scale of billions of tons per year, at low cost, with low environmental impact and greenhouse-gas absorption.*
- *Arrays of artificial APPN modules organized in factory-style architectures will enable fabrication of AP products on all scales and from a wide range of synthetic materials: photovoltaic cells, fuel cells, CPUs, displays, sensors, therapeutic devices, smart materials, etc.*
- *Across a wide range of devices and systems, pursuing the ultimate in high performance drives toward atomic precision, as only atomic precision can enable optimal structures.*

Atomically precise productive nanosystems (APPNs) are nanoscale APM systems that are themselves atomically precise. Biological APM systems are all APPNs. As APM technologies are drawn upon to work with a wider range of materials, APPNs will become applicable to wider and wider ranges of products. This will lead to materials and devices of unprecedented performance.

Robust physical scaling laws indicate that advanced systems of this type can provide high productivity per unit mass, and requirements for input materials and energy should not be exceptional. These considerations and experience with the bio-based APPNs suggest that products potentially can be made at low cost. With further development and scale-up at the systems level, arrays of APPNs will be applicable to the production of streams of components that can be assembled to form macroscale systems. These characteristics of scale, cost, and performance point to far-reaching, disruptive change that spans multiple industries.

No alternative to APPNs has been suggested that would combine atomically precise production of complex structures with the potential for cost-effective scale-up. APT development leads toward unique opportunities.

The Roadmap Workshops Opened a Unique Window on the Potential of APT

The Roadmap project provided a unique, cross-disciplinary process for exploring current capabilities and near-term opportunities in APT, and explored pathways leading toward advanced APM. Our inaugural meeting, held in San Francisco, was followed by workshops at the Oak Ridge, Brookhaven, and Pacific Northwest National Laboratories. These meetings were unusual in the breadth of disciplines and research experience brought by the participants. They were unique in their focus on integrating knowledge applicable to the development of APT and APM.

Workshop participants gained new perspectives and directions for their research. The body of this Roadmap document brings together threads from the meetings and subsequent exchanges, pointing to research directions that promise remarkable rewards.

APM Products Will Have Broad and Growing Applications

Potential products of APM are applicable to familiar nanotechnology objectives in energy production, health care, computation, materials, instrumentation, and chemical processing. These include:

- Precisely targeted agents for cancer therapy
- Efficient solar photovoltaic cells
- Efficient, high-power-density fuel cells
- Single molecule and single electron sensors
- Biomedical sensors (*in vitro* and *in vivo*)
- High-density computer memory
- Molecular-scale computer circuits
- Selectively permeable membranes
- Highly selective catalysts
- Display and lighting systems
- Responsive ("smart") materials
- Ultra-high-performance materials
- Nanosystems for APM.

The most attractive early applications of APM are those that can yield large payoffs from small quantities of relatively simple AP structures. These applications include sensors, computer devices, catalysts, and therapeutic agents. Many other applications, such as materials and energy production systems, present greater challenges of product cost or complexity. There is likewise a spectrum of challenges in required materials properties and durability in application environments. Early niche applications can provide momentum and market revenue, and we anticipate that ongoing improvements in product performance, complexity, and cost will ultimately enable the full spectrum of applications outlined in the Roadmap, as well as applications yet to be imagined.

Call to Action for APT Advancement

This Roadmap is a call to action that provides a vision for atomically precise manufacturing technologies and productive nanosystems. The United States nanotechnology advancement goal should be to lead the world towards the development of these revolutionary technologies in order to improve the human condition by addressing grand challenges in energy, health care, and other fields. The United States can accomplish this goal through accelerated global collaborations focused on two strategies that will offer ongoing and increasing benefits as the technology base advances:

1. Develop atomically precise technologies that provide clean energy supplies and a cost-effective energy infrastructure.
2. Develop atomically precise technologies that produce new nanomedicines and multifunctional *in vivo* and *in vitro* therapeutic and diagnostic devices to improve human health.

Atomically Precise Technology (APT)

- *Atomic precision is the guiding vision for nanotechnology.*
- *Required for Moore's law progress in 15 year time frame.*
- *Required for optimal materials and systems.*
- *Current forms have sharply restricted capabilities.*
- *Advances will enable expanding applications.*
- *APT development requires focused cross-disciplinary research to develop a body of engineering knowledge for systematic design and improvement of AP nanosystems.*

The vision expressed in this Roadmap is to use nanotechnology to improve the human condition. We believe that the most cost-effective way to do this is to develop atomically precise technologies and productive nanosystems, which enable science, engineering, and manufacturing at the nanoscale. To justify the investment, the long-term development pathway must have intermediate milestones that demonstrate real benefits.

Close cooperation between government, academia, and industry is necessary to cover the spectrum from basic to application-oriented research. To foster the necessary breakthroughs, participating universities must develop advanced study programs that address productive nanosystems. Long-term and high-risk research will require investment by government and philanthropic sources, since industry can seldom afford to invest in such research. However, an efficient approach to developing and commercializing technologies based on productive nanosystems must foster competition, since market competition has repeatedly proven to be the most efficient way to allocate the ever-scarce resources of talent, time, and money. In all areas, we must measure our success by results, not by dollars spent.

Close cooperation among scientific and engineering disciplines will be necessary because of the nature of the engineering problems involved. This cross-disciplinary collaboration will bring broad benefits through the cross-fertilization of ideas, instruments, and techniques that will result from developing the required technology base.

With international cooperation, the benefits of productive nanosystems will be delivered to the world faster. Coordinating a full international effort is extremely desirable in order to minimize duplication of effort in smaller national programs conducted independently.

Recommendations

As a foundation for action, establish research objectives and organizations that will be effective in developing APT systems.

- Develop a broad technology base for APT and apply this to develop improved APM, APPNs, and spinoff APT applications. Use atomic precision as a merit criterion for general research in nanofabrication. For research directed toward APM and APPNs, treat atomic precision as an essential criterion.
- Build partnerships among research institutions to coordinate the development of complex, atomically precise

nanosystems. Complement scientific exploration of novel phenomena with engineering approaches that exploit and integrate components that exhibit more predictable behavior.

- Promote collaboration aimed at satisfying the multiple requirements for building next-generation systems. The International Technology Roadmap for Semiconductors illustrates this vital role, coordinating diverse groups to develop the comprehensive sets of tools needed to fully enable next-generation technologies.

Support work on modeling and design software that facilitates AP nanosystem development.

- Prioritize modeling and design software as critical elements in the development and exploitation of APM, APPNs, and spinoff APT applications.
- Support ongoing research in multi-scale modeling to describe physical phenomena in large systems at different levels of theory and resolution. Focus this research on requirements needed to support computer-aided design software for AP nanosystems.
- Develop software that addresses domain-specific problems of modeling and design in diverse classes of AP nanosystems, including structures made by tip-directed APM and by the folding and AP self-assembly of nanoscale polymeric objects.
- Develop compilations of data organized to support design and implementation of APT systems. Classify materials, building blocks, devices, and processes, enabling search according to criteria and metrics that describe their functional characteristics. These compilations will cut across the disciplinary barriers that now impede the flow of practical knowledge.

Develop tools and processes to support tip-directed APM.

- Develop stable, reproducible, atomically precise scanning tunneling microscope tips.
- Develop tool tips that capture and transfer atoms, molecules, or other building blocks in known configurations; tool tips able to sense building-block capture and release.
- Develop closed-loop nanopositioning systems with resolution < 0.1 nm and three or more degrees of freedom;

Atomically Precise Manufacturing (APM)

- *Essential feature: programmable control of operations.*
- *Required for engineering and fabricating complex AP systems.*
- *Scanning probe devices: APM on metals, semiconductors.*
- *Biomolecular machines: APM of polymer objects.*
- *Self-assembly: large AP products from smaller ones.*
- *Near-term APM promises a growing range of applications.*
- *Advanced APM promises revolutionary applications.*

develop small-footprint systems to implement array-based parallelism

- Improve atomic layer epitaxy and atomic layer deposition.
- Seek means for highly selective depassivation and etching of surfaces and for atomically precise functionalization.
- Seek means for direct placement and bonding of atoms and molecules and for atomically precise defect inspection, repair.
- Develop robust protection layers to preserve the atomic precision of APM products.

Atomically Precise Productive Nanosystems (APPNs)

- *Essential feature: APM processes implemented by APFNs.*
- *Bio-APPNs are the central fabrication systems in living cells.*
  - *Used in biotech for bulk production: 10^{10} to $>>10^{20}$ units.*
  - *Can now design and make 3D, 10^7-atom biopolymer objects.*
- *Advanced-generation APPNs provide a road forward.*
  - *Bootstrap the capabilities of next-gen APPNs.*
  - *Expand range of materials: ceramics, semiconductors, metals.*
  - *Increase performance of components for APFNs*
  - *Robust scaling laws predict high throughput per unit mass.*
  - *APPN arrays enable macroscale products from nano parts.*

Expand and exploit sets of building blocks for AP self- and tip-directed assembly.

- Explore and catalog diverse sources of AP components: natural and synthetic molecules, AP nanoparticles, DNA and protein objects, products of tip-directed APM.
- Expand the set of atomically precise building blocks for both AP self assembly and tip-directed methods.
- Develop monomeric building blocks for ribosome-like synthesis of AP polymer sequences with subsequent folding, binding, and cross-linking to form AP polymeric objects by self-assembly.
- Develop prototype APPNs that perform ribosome-like synthesis of AP polymer sequences.
- Make atomic precision a criterion for APT-relevant self-assembly research.
- Make systematic design methodologies a merit criterion for research in AP self-assembly.

Support the development of modular molecular composite nanosystems (MMCNs).

- Extend and exploit the recent development of configurable, 3D, million-atom-scale DNA frameworks with dense arrays of distinct, addressable, AP binding sites.
- Extend and exploit the capability of protein engineering to produce functional, relatively rigid AP polymer objects.
- Expand capabilities for engineering proteins with AP binding to DNA frameworks and functional components.

- Develop systematic methodologies for building MMCNs in which proteins bind specific functional components to specific sites on DNA structural frameworks.
- Support theoretical and experimental research to develop and exploit the ability to organize large numbers of distinct, functional nanostructures in 3D patterns on a 100 nm scale.
- Develop means to interface MMCNs with nanostructured substrates patterned by tip-directed AP fabrication and by non-AP nanolithography.
- Pursue synthetic biology approaches for bringing the cost of DNA into line with the cost of proteins and other biopolymers.

Some Enabling Technologies

- *Structural DNA nanotechnology*
- *Scanning probe manipulation*
- *Protein design*
- *Macromolecular self assembly*
- *Nanoparticle synthesis*
- *Nanolithography*
- *Organic synthesis*
- *Biotechnology and molecular biology*
- *Surface science*
- *Molecular imaging*

Explore objectives for system development.

- Extend and exploit methodologies for using modeling and design to specify APT systems well enough to indicate the requirements for their implementation.
- Use these methodologies to identify research objectives that can reasonably be anticipated to have high payoff.
- Develop objectives and requirements for implementing high-payoff APT systems, including both APT applications and next-generation APM and APPN technologies that will expand the range of APT applications.

Looking Forward

This initial roadmap explores a small part of a vast territory, yet even this limited exploration reveals rich and fertile lands. Deeper integration of knowledge already held in journals, databases, and human minds can produce a better map, and doing so should be a high priority. Some research paths lead toward ordinary applications, but other paths lead toward strategic objectives that are broadly enabling, objectives that can open many paths and create new fields. These paths are the focus of this roadmap. They demand further exploration.

Looking forward, we see both incremental payoffs and grand challenges that can be achieved through a chain of strategic objectives. Advancing from exploration, to pioneering, to full exploitation will require a great effort, but this will be a natural progression. Great rewards are already visible. They merit a commensurate investment.

Technology Development and Applications Overview

Development Area	Horizon I
Atomically Precise Fabrication and Synthesis Methods	• Bio-based productive nanosystems (ribosomes, DNA polymerases) • Atomically precise molecular self-assembly • Tip-directed (STM, AFM) surface modification • Advanced organic and inorganic synthesis
Atomically Precise Components and Subsystems	• Biomolecules (DNA- and protein-based objects) • Surface structures formed by tip-directed operations • Structural and functional nanoparticles, fibers, organic molecules, etc.
Atomically Precise Systems and Frameworks	• 3D DNA frameworks, 1000 addressable binding sites • Composite systems of the above, patterned by DNA-binding protein adapters • Systems organized by tip-built surface patterns
Applications	• Multifunctional biosensors • Anti-viral, -cancer agents • 5-nm-scale logic elements • Nano-enabled fuel cells and solar photovoltaics, • High-value nanomaterials • Artificial productive nanosystems

Horizon II	Horizon III
• Artificial productive nanosystems in solvents • Mechanically directed solution-phase synthesis • Directed and conventional self-assembly • Crystal growth on tip-built surface patterns • Coupled-catalyst systems	• Scalable productive subsystems in machine-phase environments • Machine-phase synthesis of exotic structures • Multi-scale assembly • Single-product, high-throughput molecular assembly lines
• Composite structures of ceramics, metals, and semiconductors • Tailored graphene, nanotube structures • Intricate, 10-nm scale functional devices	• Nearly reversible spintronic logic • Microscale 1 MW/cm^3 engines and motors • Complex electro-mechanical subsystems • Adaptive supermaterials
• Casings, "circuit boards" to support, link components • 100-nm scale, 1000-component systems • Molecular motors, actuators, controllers • Digital logic systems	• Complex systems of advanced components, micron to meter+ scale • 100 GHz, 1 GByte, 1 μm-scale, sub-μW processors • Ultra-light, super-strength, fracture-tough structures
• Artificial immune systems • Post-silicon extension of Moore's Law growth • Petabit RAM • Quantum-wire solar photovoltaics • Next-generation productive nanosystems	• Artificial organ systems • Exaflop laptop computers • Efficient, integrated, solar-based fuel production • Removal of greenhouse gases from atmosphere • Manufacturing based on productive nanosystems

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