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Balancing the National Nanotechnology Initiative's R&D Portfolio

A Foresight/IMM White Paper submitted to the
White House Office of Science and Technology Policy*

Neil Jacobstein, Ralph Merkle, Robert Freitas

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The National Nanotechnology Initiative (NNI) defines "nanotechnology" as research and technology development in the length scale of approximately 1 to 100 nanometers. **This White Paper proposes that the portfolio of NNI research and development projects should be balanced periodically to ensure a range of low-, medium-, and long-term projects, as well as a wider range of risk. Given the recent interest of the venture capital community in nanotechnology, it would make sense to focus more NNI projects on high-risk, high-payoff R&D that would be outside the time horizon of the private sector. This action would be consistent with the need to increase the performance and accountability of federally funded research programs.**

In a fundamental sense, the NNI is charged with expanding our technological capabilities for manufacturing, and addressing the question of what arrangements of atoms are possible and are desirable to make. Thus the NNI accelerates trends in manufacturing dating back centuries or more. The ultimate limits are dictated by basic physics and economics, and may be defined in terms of what is possible:

- Flexibility: arranging atoms in most of the ways permitted by physical law.
- Quality: getting almost every atom in the right place (> 7 sigma quality levels).
- Cost: manufacturing at increments above the expense of raw materials.

If the U.S. could manufacture large-scale products with high flexibility, high quality, and extremely low cost, it would possess an economic driver much larger than the whole of computing technology in the last quarter century. This is not an exaggeration, nor is it a description of a free lunch. It is the recognition of an economic opportunity that will accrue to any country that develops molecular manufacturing first.

* This summary paper was requested as a follow-up to a series of meetings with the OSTP in early 2002.

However, developing molecular manufacturing will be difficult. It requires a time perspective beyond the usual commercial and industrial R&D horizons. It will take long-term R&D funding that is focused on specific and accountable performance objectives. This fits the high-risk, high-reward profile for federally funded R&D. However, unlike projects that are essentially "science experiments" with unknown or unaccountable outcomes or performance objectives, we already know that molecular manufacturing of large objects at little more than the cost of raw feedstock is possible because it happens in nature. For example, trees are solar-powered molecular manufacturing systems that convert the raw feedstock of soil and atmospheric carbon dioxide (CO_2) into tons of wood.

The existing charter of the NNI covers the development of molecular manufacturing systems. Would such systems prove practical? What might they look like? How might we develop them? What are their realistic economic, security, and environmental consequences over the next one to three decades? **The NNI should focus a modest percentage of its overall funding on examining their feasibility.**

Besides focusing a certain amount of effort specifically on the molecular manufacturing objective, existing research can be evaluated using an additional criterion: how does this research contribute to the development of molecular manufacturing systems? While it might not always be clear whether a specific line of research would ultimately play a role in this development, some areas of research seem clearly relevant. Their potential contribution to this objective would be an additional favorable factor in determining their value.

Time Frames

Molecular manufacturing systems are likely to take longer to develop than the usual five to ten year time horizon of the private sector. The private venture capital sector has shown considerable enthusiasm for funding nanoscale science and engineering projects that focus on novel electrical or physical properties of nanoscale materials. But they are not focusing on the high-risk, high-payoff opportunity of developing molecular manufacturing components and systems with moving parts. There are some European and Japanese initiatives to develop molecular manufacturing components and systems. **The key rationale for U.S. government funding is that molecular manufacturing might not happen first in the U.S., or will happen much more slowly in the U.S., if we rely on the private sector for initial R&D stage funding. The question of who develops this technology first has profound economic, security, military, and environmental significance.** Existing NNI documents outline the potential impact of the technology in each of these areas.

A successful molecular manufacturing system that might be deployed in the 2020s could be described and analyzed today. Such a system would almost certainly be composed mostly of systems and subsystems that are not experimentally accessible at present, for the simple reason that we cannot yet build the relevant components. But if we need to think about and analyze systems that we cannot build today, and if we are to do so with any certitude, then we must initiate a carefully conceived theoretical and computational R&D program expressly for this purpose. Existing tools in computational chemistry can be harnessed to analyze molecular structures whether or not those structures are immediately buildable. Computational modeling of known experimentally accessible structures gives us confidence about the capabilities (and limits) of the modeling software, and permits us to evaluate structures that have not yet been made – and perhaps cannot directly be made – using our current 20th century technology base.

The value of such theoretical and computational work, particularly when used to assess systems that exceed our immediate experimental capabilities, is sometimes debated. But the alternative is to abandon active investigation of systems and structures that cannot be built today. **Inability to think systematically about what cannot yet be built is very likely to delay our ability to build it. If we are to build molecular manufacturing systems in the next few decades – systems that are experimentally inaccessible today – then methodical design work on such systems is both necessary and urgent.**

Systems

Another issue is the need to develop and analyze *systems*. The existing evaluation of scientific research is effective in considering specific issues, but is much less effective in generating (possibly complex) systems proposals for engineering assessment and analysis. The story of the scientist who *discovers* some new and useful property of matter after accidentally leaving the Bunsen burner turned on while away at lunch is well known. But the story of the engineer who accidentally *develops* a computer or Saturn V booster is not only unknown, but seems remarkably unlikely.

If the successful development of molecular manufacturing *systems* requires the design of complex systems (and some proposals call for the design of self-replicating systems) then we need to explicitly create programs that solicit systems proposals – proposals that can reasonably be expected to fulfill the goals of molecular manufacturing as outlined above. Systems proposals can be analyzed by theoretical and computational tools that examine the systems as a whole, together with the sub-systems and components from which they might be composed.

Management Support

Any complex team effort requires the support of management for its success. **Adding a focused effort on molecular manufacturing to the NNI will require the active support of current and future leadership.** Serious consideration should be given to the personnel who will strive to make this focused effort a success.

Metrics

There are two classes of work to be assessed: first, near-term experimental efforts to expand our capabilities, and second, theoretical and computational efforts to explore systems designs, along with their potential implementation pathways.
Existing mechanisms for evaluating experimental research are effective, but lack focus on specific molecular manufacturing targets. Specific targets that would be useful in judging the progress of the overall experimental program include: (1) positional assembly at the molecular scale, (2) nanoscale positional devices and mechanical systems, and (3) achieving mechanical performance objectives such as those specified by the Feynman Grand Prize.

The evaluation of theoretical systems designs by proposals and review in the normal channels should be effective if the objectives and metrics of these systems have support in the review community. **Metrics for these systems should focus on specific progress in developing: (i) molecular assembly and positioning devices, (ii) systems designs for achieving scalability (e.g., assemblers), (iii) control and communication systems for molecular manufacturing, (iv) energy and materials transport mechanisms, (v) embedded safeguard systems, and (vi) high value application systems.**

Three criteria are most critical when assessing molecular manufacturing R&D proposals: (A) timeliness, (B) relevance, and (C) quality.

(A) Timeliness criteria for the proposed work include: (1) Does the proposed work take account of current research and realistic milestones for progress? (2) Does it add incrementally to the body of theoretical or experimental work on molecular manufacturing available today, and if so, how? (3) Does it provide opportunities for incremental benefits prior to a complete system success?

(B) Relevance criteria for evaluating proposals include: (1) Does the proposed work focus on moving molecules with atomic precision? (2) Does it focus on developing building blocks or systems of nanoscale components? (3) Does it employ nanoscale components to move the target molecules? (4) Does the systems design work focus on any of the key molecular manufacturing design challenge areas, specifically: (i) molecular assembly and positioning devices, (ii) systems designs for achieving scalability (e.g., assemblers), (iii) control and communication systems for molecular manufacturing, (iv) energy and materials transport mechanisms, (v) embedded safeguard systems, and (vi) high value application systems?

(C) Quality criteria for proposed system evaluations include: (1) What is the depth, technical qualifications, and diversity of the research team? (2) Does the systems design team include computational chemistry and systems engineering expertise? (3) Does the proposal clearly articulate the design objectives and assessment criteria? (4) Can proposed designs be simulated or checked quantitatively? As long as the research target is unambiguously identified as molecular manufacturing, the quality of experimental work can be judged by standard criteria.

Molecular manufacturing systems designs can benefit from a detailed analysis and review by the computational chemistry community and by the systems engineering community. Proposals for molecular manufacturing systems, subsystems, and components can be taken more seriously after they have survived a broad-based review and open feedback process. A corollary of the need for this type of review is that adequate resources must be made available – in particular, an increase in funding for computational chemistry and systems engineering programs, specifically those focused on assessing proposed molecular manufacturing systems and their consequences.

Summary

The NNI portfolio is presently concentrated in a few areas of nanotechnology research. The portfolio does not yet span the full spectrum of R&D time frames or risk and reward. A strategically important technological objective within the charter of the NNI is the development of molecular manufacturing systems – the ultimate manufacturing technologies. This objective lies beyond the time horizons of private funding, even though these manufacturing technologies have fundamental national economic and strategic importance. These technologies will eventually make major contributions to U.S. competitiveness; to our defense, medical, and energy sectors; and to industrial flexibility. It is appropriate for the NNI to establish accountable performance metrics to assess U.S. progress in developing molecular manufacturing.

In particular, the NNI should seek to achieve a balance of low-, medium-, and high-risk projects in its portfolio by initiating a long-term, high-risk, high-payoff program focused on assessing the feasibility, consequences, and development paths of molecular manufacturing. This program would require no increase in top-line funding for the NNI. The program should incorporate a strong theoretical and computational design component to evaluate proposed molecular manufacturing systems, including subsystems and components – with the understanding that the full potential of this technology may take decades to develop while generating many incremental products along the way.

Frequently Asked Questions

Q: *What is the NNI **not** doing now?*
A: Research on molecular manufacturing and molecular assemblers. In this sense, the NNI is not currently balanced between short-, medium-, and long-term R&D, and it does not have a wide range of low-, medium-, and high-risk, high-payoff projects.

Q: *Aren't molecular assemblers technically infeasible?*
A: Some credible scientists think so, but to date we have not identified any technical reason to believe that the issue is feasibility rather than simply the time frame for development. The velocity of development is directly affected by research funding in countries around the world.

Q: *Why is R&D on molecular manufacturing important?*
A: Much of the long-term promise of nanotechnology used to justify the NNI is based on the prospects for molecular manufacturing. The positive consequences of molecular manufacturing will eventually include zero emission manufacturing with carbon sequestration, new security and military technologies, less expensive and high quality consumer goods, new transportation systems, and fundamentally novel medical devices. However, these powerful capabilities could also be misused unintentionally or abused deliberately – thus, the need to develop effective control systems proactively.

Q: *What changes to the objectives of the NNI are proposed?*
A: Just one: Increasing the focus on laboratory work on molecular machine system development in aid of mechanical molecular assembly, and adding theoretical design studies of molecular assemblers, in order to explore their technical feasibility, safeguards, and the consequences of the molecular manufacturing which they would enable.

Q: *Will this require a top-line budget increase?*
A: No. It will only require balancing the portfolio of programs in the NNI from time to time. This is a normal and appropriate action to take every few years.

Q: *How should the quality of the new projects be judged?*
A: The White Paper provides metrics for three criteria which are particularly critical to evaluating molecular manufacturing R&D proposals: timeliness, relevance, and quality.

Q: *What are some reasonable near-term milestones with which to judge progress?*
A: Milestones should measure progress in developing molecular assembly and positioning devices, system designs for achieving scalability (e.g., assemblers), control and communication systems for molecular manufacturing, energy and materials transport mechanisms, embedded safeguard systems, and high value application systems.

Q: *How might this new direction be announced?*
A: This balanced NNI portfolio direction could be made public via an OMB-OSTP R&D guidance letter and the President's FY2004 budget proposal.