CRITICAL NATIONAL NEED IDEA

Engineering Quantum Engineering: Manipulating atoms and molecules for practical applications

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Introduction

Quantum Engineering refers to techniques and methods utilized for the efficient manipulation of atoms and molecules for practical purposes. The manipulation and control of isolated single neutral atoms and their interactions has been a long term goal with important practical applications in many areas of interest in nanotechnology, communications, quantum engineering, fundamental physics, chemistry, and quantum computing. Since scientists begun studying ways to trap, cool and control atoms and molecules at the quantum level researchers and engineers have envisioned using them for the development of numerous exciting possible applications, from investigating novel nanomanufacturing methods and the practical exploitation of the unique quantum properties of atoms and molecules for sensors and quantum materials to the development of quantum computers and the efficient manipulation of quantum information.

Although researchers have been investigating techniques of quantum control to enable the manipulation and study of single trapped atoms and their chemical interactions with unprecedented detail studies are yet to focus on the development of their practical applications (see sections below). The engineering and scientific tools to be developed using the methods of quantum control will enable the development of numerous applications and promote, at the same time, to maintain the country's technological supremacy. The engineering of the techniques to efficiently manipulate the quantum nature of matter for the development of novel applications in nanotechnology and engineering is an area of high-risk high-reward research that has the potential to inhibit the future growth of the technological and scientific well-being of the nation if not tackled on time. This white paper introduces "Quantum Engineering" as area of national critical need and describes the potential benefits, needs, rewards, and the justification for a strong government and scientific attention. The sections below describe the scientific, technological, economic, and social advantages of performing research in this area that has potential applications in a wide variety of areas of critical need. The present paper is a description of a societal challenge in an area of critical need that must be addressed if the U.S. is to maintain its technological advantage and support the advancement of technology for the next generation. The paper is divided in three main sections that address the three main selection criteria required in the TIP program at NIST: Maps to administration guidance, Justification for government attention, and Essentials for TIP funding.

A: Maps to Administration Guidance

In recent years, in accordance with the National Nanotechnology Initiative [1,2], there is an increasing interest to perform studies in which the three-dimensional position of single isolated atoms and their interactions are under complete experimental control. Developing engineering systems that can efficiently manipulate matter at the quantum level opens possibilities for using them for a diverse range of technological applications, from developing novel practical quantum engineering technologies to manipulate matter at the atomic level for practical applications and building three-dimensional nanomaterials and nanostructures atom by atom to developing novel quantum sensors, and the efficient processing of quantum information. This type of engineering systems will certainly also find practical applications in the study of basic physics, chemistry, atom-atom interactions, and quantum dynamical processes with unprecedented detail. The practical quantum manipulation of matter and the engineering of such techniques have potential applications in many vital areas of national need such as energy, health, communications, methods for manufacturing and processing of nanomaterials, and medicine, to name a few. Developing engineering systems to develop the practical applications of the quantum manipulation of matter fits within the nanomanufacturing program component of the NNI [3] which is aimed at enabling scaled-up, reliable, and cost-effective manufacturing of nanoscale materials, structures, devices, and systems from the bottom-up.

Techniques to manipulate matter at the atomic and molecular levels have been developed over the years since the techniques to cool and confine atoms were introduced [4], but these techniques still remain within the laboratory and the practical development of their potential applications has not been possible due to the problematic nature of bringing such techniques into scale-up systems and the efficient monitoring of the processing of atoms and molecules. If the potential benefits of the quantum manipulation of matter are to become a reality there is a fundamental need to develop the quantum-engineering techniques to make them feasible. This is a societal need that needs to be addressed to harvest the benefits that research in nanotechnology, quantum sciences, and AMO Physics (atomic, molecular, and optical physics) have produced over the years.

Nanotechnology has already been identified as an area of critical national need [1-3] and the engineering of quantum engineering systems, as proposed here, fits well within the objectives of National Nanotechnology Initiative [2]. The engineering of the quantum techniques to manipulate atoms and molecules will make the development of the practical applications that the quantum manipulation of matter has to offer a possibility and represents a unique opportunity for enhancing and maintaining the technological advancement of the nation.

There is currently an increasing interest in studies in which single isolated atoms need to be under complete experimental control, both in location and arrival time. This interest is motivated in part by nanotechnology, where ever-shrinking nanoscale devices are rapidly approaching the atomic scale, and deterministic placement and interaction control of single atoms is becoming a necessity. Further motivation comes from recent developments in the quantum control of cold atoms [5-15] and quantum engineering [16-18], where proposed architectures to develop new quantum technologies and manipulate quantum information require unprecedented control over isolated quantum systems containing single atoms and molecules. Another source of motivation comes by the need for a deeper understanding of fundamental processes in atom–atom interactions that may lead to improved techniques for the assembly of novel structures and materials at the nanometer scale. In the long term, developing quantum tools to control and monitor the position and the interaction of individual atoms and molecules at the nanometer level will: (a) foster the engineering of additional systems to investigate the practical applications of building structures and materials atom by atom, (b) directly impact the development of novel quantum engineering technologies for energy, health, and chemical applications, (c) influence fundamental studies in quantum physics and chemistry by providing them with additional tools to explore key interaction processes in atoms and molecules, and (d) motivate the direct transfer of scientific results from universities into industry. According to the National Nanotechnology Initiative [2] and other sources [19], designing new atomic and molecular assemblies on an atom-by-atom basis is expected to increase in importance over time. The technological possibilities are numerous, but we need to build the instruments and engineering techniques to make them a reality. If we are to take a step forward in this direction there is a need to develop the engineering tools and systems that can make the possible applications of the quantum control of matter a reality.

The existence of engineering techniques to control and monitor matter at the atomic and molecular scales will empower the development of new techniques in nanotechnology and facilitate the practical development of novel quantum technologies for energy, health, and chemical applications. Indeed, with the new techniques of quantum control of atoms and molecules being constantly refined, and with nanoscale devices approaching the atomic scale, new engineering instruments to control and monitor the position and dynamics of individual atoms and molecules will be fundamental in the development of new techniques to synthesize and process materials at the atomic scale.

Recently, using techniques from atom cooling and trapping, quantum control, and optical dipole traps researchers have succeeded in delivering single 'cold' atoms in deterministic ways [16-18]. These single-atom delivery techniques open the possibility to study atom-atom interactions and quantum dynamical processes in materials with an unprecedented detail. They also open possibilities for the *engineering* of these techniques for a diverse range of technological applications, from building three-dimensional nanomaterials and nanostructures atom by atom to the efficient processing of single qubits of quantum information. The engineering of these systems for potential practical applications is one of the main goals of the present area of critical need.

Besides manipulating the external degrees of freedom of isolated atoms and molecules the quantum engineering of microscopic systems will require to control their interactions with other atoms and molecules as well. The study and control of 'cold' atoms and their interactions (collisions) by optical, magnetic, and electric fields in atomic beams and traps, holding millions of atoms, have had a productive and successful history. Despite the successes made in these studies no attempts have yet been made, to our knowledge, to expand those investigations to develop practical systems involving single atoms with independent position, time, and state controls. The engineering of recently-developed techniques of quantum control to position single atoms and molecules with nanometer control while, at the same time, manipulating their internal quantum states is a novel area of research that can be used to investigate novel techniques of nano-manufacturing at the atomic and molecular levels. In these few-particle systems new fundamental processes are expected to be seen that will allow scientists to develop more precise control mechanisms for the quantum manipulation of atoms and molecules.

At present major challenges for the engineering development of quantum techniques to control atoms and molecules that can be applied for the direct development of practical applications still exist, for example (a) the engineering of quantum engineering systems that will allow a more practical approach to the control of single atoms and molecules, (b) the development of practical control mechanisms that affect the interactions when one works with individual particles, (c) the investigation of novel nano-manufacturing techniques of structures at the atomic level using quantum control techniques of single atoms and molecules, and (d) the development of techniques to precisely measure the position of individual atoms and molecules in all three-dimensions in space and time. The precision measurement of position and localization of atoms in three-dimensions, for example, is of great interest for numerous applications and for investigating the three-dimensional assembly of structures at the atomic scale.

B: Justification for Government Attention

The engineering of systems to manipulate atoms and molecules at a practical level represents a mayor step in nanotechnology. According to the National Nanotechnology Initiative [1] the ability to control matter at the atomic and molecular scales will constitute a basic fabric of the technology of the world in which we live and work I the years to come, its importance will increase in the years ahead. The quantum manipulation of matter will play a mayor role for shaping many of the technologies that affect our lives and work environments. The U.S. risks loosing its technological advantage if such technologies are not developed. The U.S. is not the only nation that is investing in nanotechnology R&D [2,3]. In addition to Japan and Europe (through spending by individual nations and by the EU), many other countries have organized initiatives in developing the applications that quantum science promises. Russia has recently established a program based closely on the U.S. model to do research in nanotechnology initiatives and intends to spend $1.4 billion a year on nanotechnology research alone, with part of it going to research efforts in the practical applications of quantum science and the control of matter at a fundamental level.

Besides the direct applications to nanotechnology, in the long term, developing efficient quantum engineering tools and techniques to control the position and the interaction of individual atoms and molecules at the nanometer level will: (a) foster the *engineering* of additional systems to investigate the practical applications of building structures at the atomic scale, (b) directly impact the development of novel quantum engineering technologies, (c) influence fundamental studies in quantum physics and chemistry by providing them with additional tools to explore key interaction processes in atoms and molecules, and (d) motivate the direct transfer of scientific results from universities into industry. Likely proposers to submit applications in this area, hence, include scientists and engineers from academia, national laboratories, and industry, all of whom can make important contributions and give refreshing perspectives from different points of view.

According to the report "Productive Nanosystems: A Technology Roadmap", published in 2007 [3], atomically precise technologies (APT) hold the potential to meet many of the greatest global challenges, bringing revolutions in science, medicine, energy, manufacturing, communications, electronics, and industry. The *Technology Roadmap* report [3] points the way for strategic research initiatives to deliver on this promise.

Atomically precise technologies are 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.

The challenge is now, besides building and expanding on the achievements done so far in the quantum manipulation of atoms and molecules, to work on the next steps to develop the practical applications that the quantum manipulation of matter has to offer to enable the production of a larger range of atomic structures and provide more powerful APT systems of larger scale, greater complexity, 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). Atomically precise manufacturing processes use a controlled sequence of operations to build structures with atomic precision. Scanning probe devices achieve this on crystal surfaces but more complex systems need to be built to accomplish this in three dimensions and fully develop the potential applications of the quantum manipulation of matter.

Recently identified approaches for using products of APM to organize and exploit other functional nanoscale components show great promise, and quantum engineering systems are some of them. Building on achievements in quantum science, they point to capabilities that could prove transformative in multiple fields, expanding the set of nanoscale building blocks and architectures for new research products and materials. 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 suggest that products potentially can be made at low cost. With further development and scale-up at the systems level, arrays of quantum engineering systems will be applicable to the production of streams of components that can be assembled to form specific technologies, nanoscale systems, and control chemistry at the nanoscale level, to name a few. These characteristics of scale, cost, and performance point to far-reaching technologies that can span multiple industries.

No alternative to quantum engineering systems has been suggested that would combine atomically precise manipulation of atoms and molecules with the potential for scale-up. Quantum engineering leads toward unique opportunities.

Potential future products of the manipulation of matter at the quantum level are applicable to many familiar nanotechnology objectives in computation, materials, instrumentation, and chemical processing. These include:

- Single molecule and single atom sensors
- Biomedical quantum sensors (*in vitro* and *in vivo*)
- High-density computer memory

• Molecular-scale computer circuits
• Quantum computers
• Efficient quantum information processing
• Responsive ("smart") materials
• Ultra-high-performance materials
• Nanosystems for APM.

The most attractive early applications of quantum technologies are those that can yield large payoffs for developing many other potential applications. These applications include sensors, quantum information systems, and nanomanufacturing techniques. Early niche applications can provide momentum and market revenue, and it is anticipated that ongoing improvements in performance, complexity, and cost will ultimately enable the full spectrum of applications. These applications, however, require a strong involvement from government, academia, and industry to become a reality. Government and industry involvement are especially needed since initial progressive research efforts to develop new technologies with far-reaching social impacts always have come from recognizing the societal needs together with the economic advantages of the technologies to be developed.

C: Essentials for TIP funding

Maintaining American technological and economic competitiveness involves an "innovation ecosystem" with various components, each of which must be sustained. A critical element is strong Federal investment in R&D, such as the Technology Innovation Program (TIP), along with policies that encourage private sector research spending. The National Nanotechnology Initiative [1-3] already marks some of the policies that have been suggested to allow the U.S. to remain competitive in science and technology within the nanotechnology arena. The strong initiative in nanotechnology already supports basic research efforts in quantum science directed by investigators in academic and government laboratories but the applied research initiatives that can push the fast development of practical applications that quantum science has to offer are not yet tackled. One of the main reasons for a lack of progress in developing the practical applications that the quantum manipulation of atoms and molecules has to offer is that, despite the remarkable progress in fundamental research, they require the efforts from interdisciplinary teams of physicists, chemists, and engineers to be successful. Most research programs, however, are still weak in using the advantages of interdisciplinary research to accomplish results. The Technology Innovation Program, with its features to promote high-risk innovation programs on a cost-shared basis, has the capacity to promote the interdisciplinary research efforts needed to make advancements in this area of investigation that combines basic and applied research.

The engineering of quantum processes to control matter at the atomic and molecular levels will require close cooperation between government, academia, and industry to cover the spectrum from basic to application-oriented research. To foster the necessary breakthroughs, participating entities must develop advanced research programs that address productive quantum systems. Long-term and high-risk research will require investment by government and philanthropic sources, since industry can seldom afford to invest in such research 100% of the resources needed. An efficient approach to developing and commercializing technologies based on productive quantum systems must also 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. To stay competitive, we want to train U.S. workers to be the best and at the same time attract and retain talented and skilled individuals from around the world. Private industry has shown to be extremely efficient in these areas.

Finally, in order to convert innovation into competitive products, the business environment should encourage entrepreneurship and protect intellectual property. Policies and investments that support each of these components of the innovation ecosystem, along with a thriving investor community that provides access to capital and is willing to take risks, will enable the U.S. to remain not only competitive, but the world leader in science and technology.

Besides the direct application to materials and energy technologies, in the long term, developing efficient quantum engineering tools and techniques to control the position and the interaction of individual atoms and molecules at the nanometer level for practical applications will: (a) foster the *engineering* of additional systems to investigate the practical applications of building structures at the atomic scale, (b) directly impact the development of novel quantum engineering technologies, (c) influence fundamental studies in quantum physics and chemistry by providing them with additional tools to explore key interaction processes in atoms and molecules, and (d) motivate the direct transfer of scientific results from universities into industry. Finally, investigating the practical development of quantum technologies will also impact education by offering scientists, engineers, and students a refreshing perspective that bridges fundamental concepts in physics with the design of the quantum technologies of tomorrow. The projects that respond to this research initiative will, at the same time, develop significant new insights and applications through cross-disciplinary collaborations and will stimulate the Nation's capabilities in science and technology. As outlined in the National Nanotechnology Initiative [2,3] the development of the engineering technologies to manipulate matter at the quantum level for practical applications will impact society in a variety of ways by providing new tools that will impact manufacturing, nanotechnology, communications, quantum engineering, fundamental physics, chemistry, and quantum computing. The basic science concepts already exist and efforts can now concentrate in developing the practical applications that quantum science promises.

Final Remarks
The manipulation and control of isolated single neutral atoms and their interactions in both space and time has been a long term goal with important applications in nanotechnology, quantum engineering, fundamental physics, quantum chemistry, and quantum computing [39,40]. Designing new atomic and molecular assemblies, including new nanostructures and novel nanomaterials, on an atom-by-atom scale is expected to increase in importance over time [16]. There are at least three reasons for the current interest in atom-level nanotechnology. First, the research is helping us fill a major gap in our fundamental knowledge of matter. Second, it will create novel manufacturing techniques with many potential applications in industry, and third, it will help develop new nanostructures that will impact a wide range of technological areas as electronics, communications, medicine, information technology, and energy. Due to the nature of the area of critical need presented here, the research in this area has a direct impact in all these areas.

The techniques to be developed during the projects that respond to the research initiatives proposed here will support the development of innovative synthesis and processing techniques for nanomaterials (nanomanufacturing), the design of novel nanoscale materials, the organization of nanostructures into macroscopic structures, and the direct control of chemical processes at a fundamental level. The proposed initiatives will enable a rapid transfer of the basic techniques in quantum control into research areas that will explore their practical applications and their incorporation in industry.

The engineering of quantum engineering systems out from the laboratory environment is a tremendous task that will require support from the government if it is to reach its full potential and deliver the expectations it promises to society. It will require the support from government to bring together scientists and engineers from academia, national laboratories, and industry to work together and bridge the gaps that exist between basic and applied research in quantum science and the manipulation of atoms and molecules.

References

[1] NSTC, *National Nanotechnology Initiative: The Initiative and its Implementation Plan*, Washington DC, 142 pp, (2000) available on the Web at http://www.nano.gov/nni2.pdf , and NSTC, National Nanotechnology Initiative: Supplement to the President’s FY Budget, Washington DC (2004).

[2] The National Nanotechnology Initiative: Strategic Plan 2004, (Developed by the Nanoscale Science, Engineering, and Technology Subcommittee, the Committee on Technology, and the National Science and Technology Council)

[3] The National Nanotechnology Initiative: Strategic Plan 2007

[4] JOSA B: Special issue on atom cooling () and references within.

[5] W. Alt, D. Schrader, S. Kuhr, M. Müller, V. Gomer and D. Meschede, *Phys. Rev*. A **67**, 033403 (2003)

[6] D. Schrader, S. Kuhr, W. Alt, M. Müller, V. Gomer, and D. Meschede, *Appl. Phys*. B **73**, 819-824 (2001)

[7] S.B. Hill and J.J. McClelland, *Appl. Phys. Lett*. **82**, 3128 (2003).

[8] S. Yoon, Y. Choi, S. Park, J. Kim, J.H. Lee, and K. An, *App. Phys. Lett*. **88**, 211104 (2006).

[9] J. Ye, D.W. Vernooy, and H.J. Kimble, *Phys. Rev. Lett*. **83**, 4987 (1999).

[10] Nußmann S, Hijlkema M, Weber B, Rohde F, Rempe G, Kuhn A, *Phys. Rev. Lett*. **95**, 173602 (2005).

[11] Schlosser, N., Reymond, G. & Grangier, P., *Phys. Rev. Lett.* **89**, 023005 (2002).

[12] W. Alt, D. Schrader, S. Kuhr, M. Müller, V. Gomer and D. Meschede, *Phys. Rev*. A **67**, 033403 (2003)

[13] Doherty, A. C., Lynn, T. W., Hood, C. J. & Kimble, H. J., *Phys. Rev.* A **63**, 013401 (2001)

[14] J. Ramirez-Serrano, W. DeGraffenreid, and J. Weiner, *Phys. Rev*. A **65**, 052719 (2002)

[15] J. Ramirez-Serrano, W. DeGraffenreid, J. Weiner, E. Tiesinga, and P.S. Julienne, *Phys. Rev.* A **69**, 042708 (2004).

[16] D. Meschede, A. Rauschenbeutel, "Manipulating Single Atoms", in: Adv. At. Mol. Phys. **53**, G. Rempe and M. 0. Scully, eds., 76-105, (2006)

[17] Y Miroshnychenko, W. Alt, I. Dotsenko, L. Forster, M. Khudaverdyan, D. Meschede, D. Schrader, A. Rauschenbeutel, *Nature* **442**, 151 (2006)

[18] Y Miroshnychenko, W. Alt, I. Dotsenko, L. Forster, M. Khudaverdyan, D. Meschede, S. Reick, and A. Rauschenbeutel, *Phys. Rev. Lett*. **97**, 243003 (2006)

[19] M.C. Roco, *Nanoscale Science and Engineering: Unifying and Transforming Tools*, AIChE Journal, **50**, 890 (2004)