# Nanotechnology Research: Enabling Technologies for Innovative New Materials

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*Table of Contents*



## Enabling Technologies for Innovative New Materials

In the quest to develop new innovative products, researchers are increasingly relying on computational technologies to help simulate the properties of new materials. Ultimately, scientists engaged in materials research aim to develop new compounds that can predictably be applied to a product development program. While there are many disciplines that contribute to the research of new materials, nanotechnology research offers the greatest opportunity for developing innovative compounds to significantly enhance products and quality of life for consumers. Working at the nanometer scale ($10^{-9}$ meters), this rapidly evolving field is being used to develop numerous solutions which, like many new technologies, results in multiple definitions. Two of these distinct nanotechnology-derived fields of research are:

1. Nanoscale molecular machines that are used to build atomic scale products: While the development of these devices continues to evolve, they have been utilized for many years in fields such as modern microprocessor manufacturing.

2. Technologies that create nanoscale materials: Developing atomic-scale particles with new and previously unattainable properties. Examples of these include nanocrystalline particles in products such as sunscreens, surface coatings, and filter devices, or carbon nanotubes in strong materials.

The basis for understanding how these particles can be developed relies first in being able to model and predict the chemical reactions used to construct them. Critical to achieve this capability are the modeling tools which predict the molecular mechanics and molecular physics of these systems at the quantum theory level.

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Considered a disruptive technology, most of the historical nanotechnology research has been performed by university and government labs. However, due to the potential positive economic impact offered by new nanomaterials, major government and commercial investment around the world is now focused on developing rational nanoscale material design. Value from nanoscale products can be achieved through new capabilities including:

- Improved materials demonstrating advanced properties
  - Hardness
  - Strength
  - Heat conductivity/resistance
  - Electrical conductivity/resistance
  - Flexibility
- Improved access to new locations
  - Bloodstream
  - Space
  - Toxic Sites

Due to the immense return on investment potential, greater numbers of commercial organizations have begun to include this technology as a core development capability. Clearly, nanotechnology-based materials have the ability to provide significant advancements to a number of industries. Some of the many examples of nanomaterials can be placed into three categories:

- Delivery/Access
  - Improve drug safety and efficacy through targeted delivery
  - Deliver drug and genes into intracellular organelles
  - Emit electromagnetic energy to treat hyperthermia and eradicate tumors through thermal ablation
  - Act as targeted anti-microbial, anti-viral, and anti-fungal agents
- Sensors
  - Develop smart dust, light materials deposited into the atmosphere designed to measure various conditions
  - Enhance molecular imaging by improving contrast for use in diagnostics (e.g., the early identification of cancer cells)
  - Analyze blood components through biosensor reactions to target biomolecules
- Coatings
  - Store data on tape encoded with nano-manufactured DNA
  - Build vehicles with surfaces coated with nano-manufactured diamonds
  - Store data on manufactured diamond coated disks
  - Engrave silicon 100 times finer than current technologies with carbon nanotubules

## Molecular Modeling—The Driving Force Behind Nanotechnology Research

Although researchers have recently developed the technology required to observe and manipulate atoms directly, the ability to manufacture commercial products from these models remains elusive. Further, most of the research so far has been devoted to understanding the results of investigator-initiated exploratory research rather than from designing new materials to meet existing or newly identified needs. While a number of products on the market today have arisen from this ad hoc approach, a more rigorous scientific-based design and development process must be accomplished to achieve reliable returns from the technology. Rational nanomaterial design, a systematic approach that incorporates rigorous engineering design for commercialization, will be required to move the technology from a research problem to a viable tool used to predictably develop commercially successful products.

Successful rational design of nanomaterials can be achieved by understanding the fundamental atomic and molecular properties of the material at the nanoscale. Using advanced computational algorithms and high performance computers, models can be developed to predict and explore the fundamental relationships between a material's structure, properties, behavior, and composition. As a result, nanotechnology and its applications are currently a hot topic of discussion and debate in the computational science community.

Due to the wide range of materials studied in this field, molecular modeling and simulation include techniques that can aid in the analysis of molecules spanning a wide range of sizes. Molecular modeling for nanotechnology research can be divided into the following areas:

Quantum Mechanics—Quantum Mechanics (QM) methods estimate molecular properties from the interactions of electrons and because they are based on a fundamental equation of quantum chemistry, they are much more accurate than the models developed by Molecular Mechanics techniques. Additionally, QM methods are required if the processes under study involve the breaking and forming of chemical bonds. Due to the extremely complex analysis used in QM, the main disadvantage of this technique is that long computation times can be required to model a simple system. Significant computational resources should be accessible for meaningful calculations and the size of the system which can be studied has typically been limited by this requirement.

Molecular Mechanics—Molecular Mechanics (MM) can be used to model the structure of larger and more complex molecules than QM because it is based on a series of mathematical and classical physics assumptions. MM approximates molecular behavior by assuming that atomic bonds behave in a "ball and stick" manner and, compared to QM, these assumptions allow MM applications the ability to model larger groups of atoms. With the recent emergence of the QM/MM methods, researchers can combine the higher accuracy of QM in molecular regions deemed to be of interest and rely on MM methods to the surrounding areas.

Mesoscale Modeling—A broad term, mesoscale refers to the simulation of more than a few thousand atoms but less than billions. As the basic subunit for model development, MM uses entities greater than the molecular size and, as a result, these models can be developed over comparatively longer time intervals than QM and MM. This feature allows for the study of complex materials including liquids and polymers on the nanometer to micron scale. However, due to the larger scale subunit, there is a tradeoff in the accuracy of these models.

## SGI Solutions—Empowering the Nanotechnology Scientist to Innovate

To build a computing infrastructure that supports high-performance rational nanotechnology research, it is critical that a flexible and enabling high-performance solution platform is chosen. Whether in basic nanotechnology research or in commercial production, today's reality is that computing solutions are typically restricted to systems based on high-volume microprocessors combined with the now-standard open source Linux® operating system. Despite these restrictions, there are numerous choices, and a careful assessment of various parameters should be considered before making a computational system decision. These include:

- The size and nature of the problem
- The number of users working on the problem or on the research team
- Size of data and how data is accessed (e.g. disk access vs. resident in memory)
- Size of primary, intermediate, and final data (scratch data is often much larger than primary and final data)
- Available data management solutions for the platform
- Type of computational power needed to provide useful turnaround of workload
  - Type of math needed in calculations (e.g. integer vs. floating point)
  - Capability to compute large models on 32-bit vs. 64-bit environments
  - Transfer speed of connection between components (memory bandwidth). Many of the most relevant compute intensive algorithms place a heavy burden on the ability to transfer relatively large amounts of data between the memory subsystem and the processor and between processors. In addition, often the transfer bandwidth to and from peripherals like the I/O subsystem may become performance bottlenecks.
- Requirement for and availability of scalable visualization for the platform
- Development environment to support custom algorithms where needed

Based on the Intel® Itanium® 2 Processor, the SGI® Altix® is an excellent choice for nanotechnology computational research because it satisfies the requirements for a standard microprocessor-based system running Linux and offers unique capabilities that will support state-of-the-art R&D. Most of the popular applications used for nanomaterials research are ported to the Altix platform, and many have been tuned for optimized performance on the system.

The Intel Itanium 2 Processor is based on the Explicitly Parallel Instruction Computing or EPIC architecture. Since the instruction set is explicitly parallel, the architecture attains high levels of parallelism inside the processor (so called "instruction level parallelism"). Leveraging the EPIC architecture of the Itanium 2 Processors, the Altix adds parallel system architecture, an optimized set of internal resources, higher bandwidth processing, I/O and memory, delivering industry leading performance to compute-intensive applications. As the basis of this system architecture, the Itanium 2 Processor offers a wide range of execution resources giving the system an enhanced ability to execute multiple instructions simultaneously.

In addition to the raw microprocessor performance offered by the Itanium 2 Processor, the 64-bit Altix offers scientists a virtually unlimited memory capability in a tightly coupled system ultra-high speed communication environment that connects the system's microprocessors, memory, visualization graphic processor units (GPUs) and other peripherals. With this capability, the scalable Altix shared-memory platform is able to perform complex simulations that, until recently, could not be even considered. Ultimately, the highly integrated Altix server and Itanium 2 Processor, together with the available programming tools needed for software to utilize these capabilities, provides optimal performance required by the applications used for nanotechnology research. And, beyond raw performance and faster online transaction processing, the Altix enables more users to access compute resources so that more jobs can be run and more users serviced in less time.

## Nanotechnology Case Study—Empowered Research with SGI Technology

To illustrate the benefits of SGI Altix Computational Chemistry solutions in a typical nanotechnology research scenario in what could be a model of a rational nanotechnology research scenario, a case study was developed involving DFT calculations with Gaussian 03 C.02[1]. In this study, three Single Walled (sw) nanotube segments consisting of 2 (15,0) units were constructed. Each tube segment contains 60 atoms in the progression from C to Si to Ge. While the number of atoms is constant, the complexity and size of the model calculation increases from C to Si to Ge due to the increasing number of electrons. Further, the C and Si have "s" and "p" electrons, whereas Ge also has electrons occupying "d" orbitals. Evaluation of various simulation scenarios spanning across atomic composition and models such as this are typical in materials research and a key capability is to be able to routinely, effectively, and quickly evaluate all possibilities. This case demonstrates how the SGI Altix provides the infrastructure for scientists to evaluate each possibility and efficiently determine the most effective model for their research need.

To perform the prototype, each nanotube was "virtually" extended by the use of the Periodic Boundary conditions (PBC) option within Gaussian. The geometry and cell size of each nanotube were first optimized using the HCTH Density Functional with density fitting and a 3-21g basis set. Subsequently a single point energy calculation was carried out with the same basis set and the rb3lyp hybrid functional. These calculations were carried out on an SGI Altix 3000 server equipped with up to 32 Itanium 2 Processors running at 1.6 GHz and with 9MB L3 cache.

Figures 1, 2, and 3 show the HOMO-isosurfaces (value = 0.004) for the three nanotube segments. The red rod in the center is the direction of the translation vector for the PBC expansion.

Figure 1: C sw nanotube

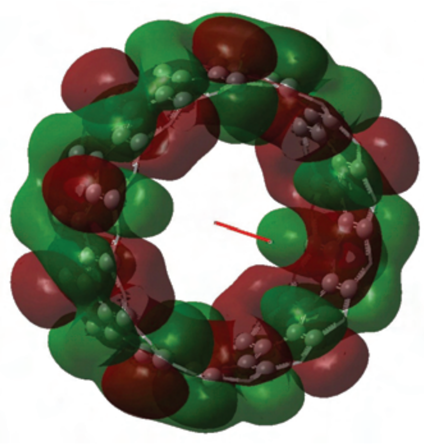

Figure 2: Si sw nanotube

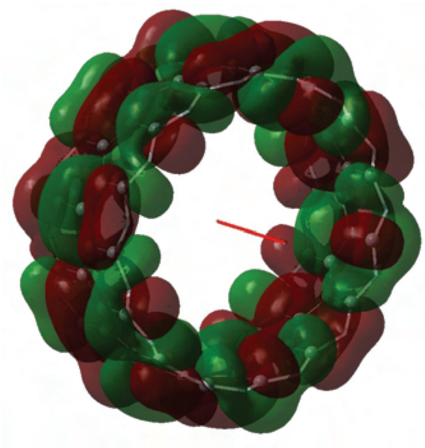

Figure 3: Ge sw nanotube

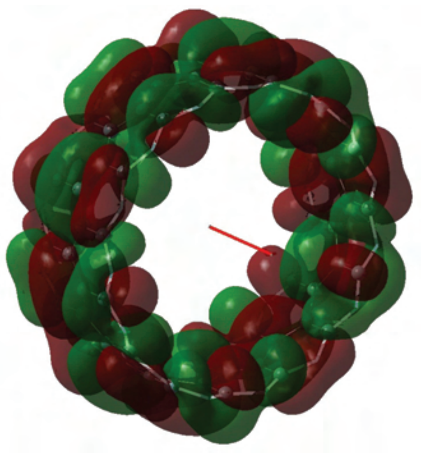

*Table 1: Time in seconds for 1 SCF cycle.*

| C | | Si | | Ge | |
|---|---|---|---|---|---|
| Basis functions | 540 | Basis functions | 780 | Basis functions | 1380 |
| Np | Time | Np | Time | Np | Time |
| 4 | 240 | 8 | 248 | 16 | 2182 |
| 8 | 139 | 16 | 115 | 32 | 1462 |

NP = Number of processors

While the C sw nanotube PBC calculation at this level of theory can easily be performed on most computer systems, the computational burden is higher for the Si sw nanotube. As demonstrated from the data below, to routinely solve the Si sw nanotube in a reasonable amount of time, a more moderately substantial computer is required. However, to perform the Ge sw nanotube model calculations, a significant high performance computer system such as the SGI Altix is required to complete the task.

With the performance tuned application, Gaussian in this case, the 32-processor Altix completes geometry optimizations and even frequency calculations for even the most challenging nanotechnology model. This case study demonstrates how the SGI Altix high-performance computing solution based on Intel Itanium 2 Processors provides scientists with the resources to readily evaluate multiple scenarios, so that the most effective nanoscale structure can be readily identified to meet their research objectives in acceptable timeframes. The case study shows that in a rational approach to this type of modeling, more computer resources can be effectively used to tackle growing problems.

## Conclusions

Nanotechnology research is an evolving field focused on developing new materials comprised of atomic scale components. To successfully develop these materials, significant computational chemistry research is required to simulate and model their properties. Depending on a model's complexity and composition, these computational simulations can require significant computational performance and, to effectively develop new nanomaterials, a scientist must be able to assess multiple options. Therefore, a high performance computing infrastructure is often required to allow scientists in this field to complete multiple "what if" scenarios so that the best model or trends in the models can be identified.

The SGI Altix family of servers based on Intel Itanium 2 Processors provides the industry's most effective computational infrastructure for nanotechnology research. The Computational Chemistry applications used in nanotechnology research require significant computational capabilities to complete simulations in a reasonable amount of time. In cases of significant simulations, less capable systems may be unable to complete the simulations at all. The industry-leading shared memory capability and high-speed connection between system components (low latency and high bandwidth) offered by the SGI Altix provides the ultimate computational resource for these applications. Further, SGI engineers have worked with the developers of the leading QM and MM applications so that they have ultimate performance and scalability on the SGI Altix family of servers. Together, these resources provide scientists with the required tools needed to enable state-of-the-art nanotechnology research.

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