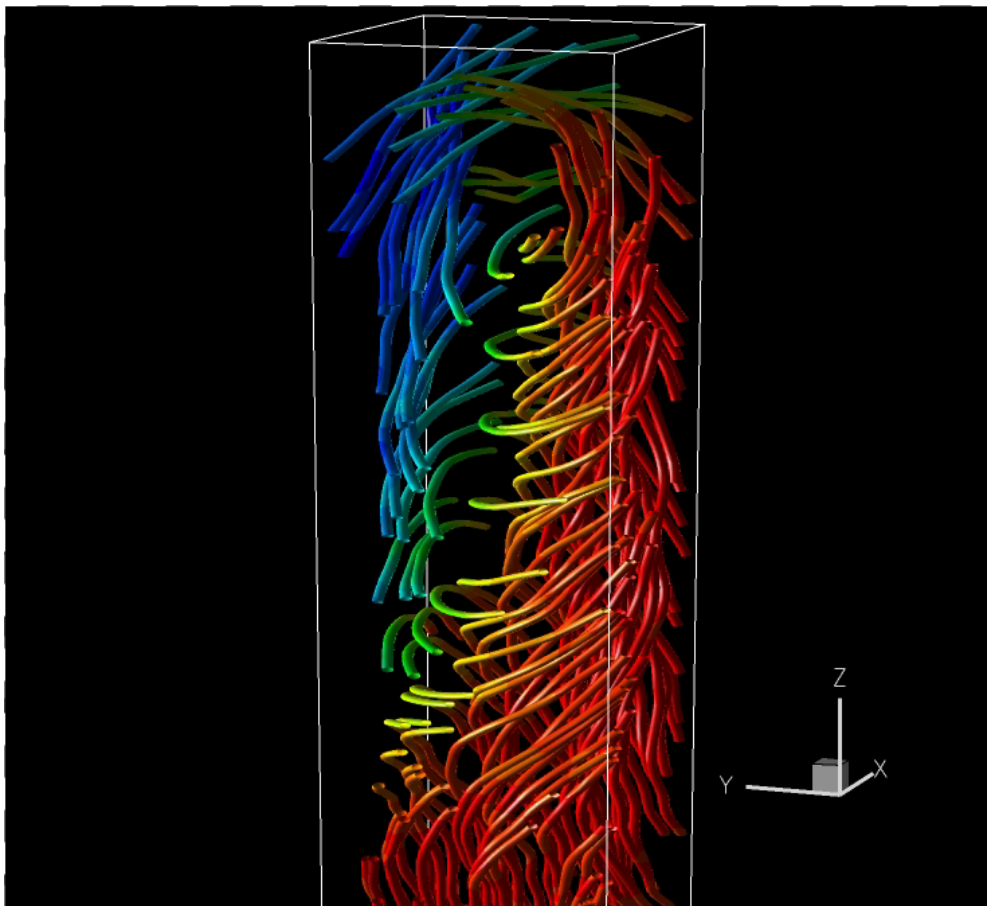
Materials Research Cyberscience

enabled by

Cyberinfrastructure



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Executive Summary

The National Science Foundation (NSF) Computational Materials Science Review was held June 17—19, 2004 at the Materials Computation Center at the University of Illinois Urbana-Champaign. 110 researchers were registered participants, including 44 PIs and co-PIs, 35 graduate students and 22 post-doctoral fellows. The first two days consisted of presentations and posters of the research performed under the NSF Division of Materials Research (DMR) Information Technology Research (ITR) grants. The purpose of this review was two-fold: first to provide an overview of the major computational activities managed by the NSF DMR, and, second, to provide input to the NSF on the cyberinfrastructure needs of the computational materials theory community to realize the potential of cyberscience in the future. This executive summary describes the recommendations to the NSF concerning the cyberinfrastructure required to continue to have DMR theory cyberscience be at the forefront of science and realize its potential contributions as a key discipline in science and technology.

For this report, cyberscience will refer specifically to the science that can be accomplished within the materials theory program of DMR in its support of the wide range of programs addressing fundamental phenomena in materials, materials synthesis and processing, structure and composition, properties and performance, condensed matter physics, and materials education. Recommendations for cyberinfrastructure will specifically mean the algorithms, models, software, networks, and computer hardware that are required to perform the cyberscience investigations of DMR theory, as well as the needs of researchers and educational opportunities in cyberinfrastructure and cyberscience.

The following section contains the Executive Summary of the recommendations, and is followed by a section on the Executive Summary of the review of current activities. A summary of the discussion concerning the recommendations in the Executive Summary comprises the main body of this report. Appendix A provides an extremely brief overview of the program of the June 2004 review. Appendix B provides the comments provided by the June 2004 participants to a questionnaire concerning DMR theory cyberscience and cyberinfrastructure.

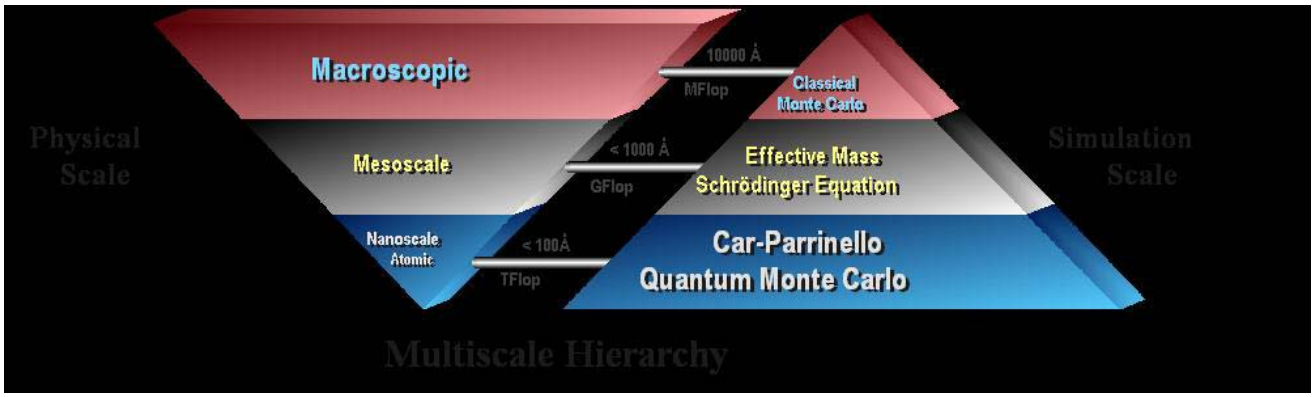

Figure 1. This illustrates the cyberscience methods for materials, from nanoscale to the macroscale, from structure to dynamics, and the required computing power from desktops to Pentaflops.

Executive Summary --- Recommendations

The recommendations by the Review participants for the cyberinfrastructure needed for cyberscience, with further details documented in this report, include:

- Continued advances in materials theory requires that the MPS directorate take the lead in providing the advanced cyberinfrastructure needed for DMR theory.
- Cyberscience, defined as science that can only be accomplished with adequate cyberinfrastructure, should be supported by MPS.
  - MPS should support computing *for* science, not computing *as* science.
  - Major discoveries are often made at the boundaries between subfields. Consequently interdisciplinary research and research groups should be encouraged.
  - Materials research has the possibility to enable new hardware thereby leading to paradigms for computing.
  - A major emphasis on education opportunities and funding for the next generation of scientists who will advance materials theory cyberscience should be undertaken.
- All aspects of cyberinfrastructure are important to perform cyberscience in materials theory, no one computational methodology or cyberinfrastructure bottleneck exists in this diverse community.
  - Algorithm and software advances are both essential for advances in science and of equal importance to equipment advances. Both should be funded, because of their importance in cyberscience. Much of the funding is in fact for human resources, with the timelines and needs different from that of equipment.
  - Access to compute power at all levels is needed for DMR materials research: single workstations, small networked clusters, as well as cycles on state-of-the-art supercomputers.
  - Access to reliable high-bandwidth networks is very important to many in the materials research community, especially for researchers not on the main network backbones.

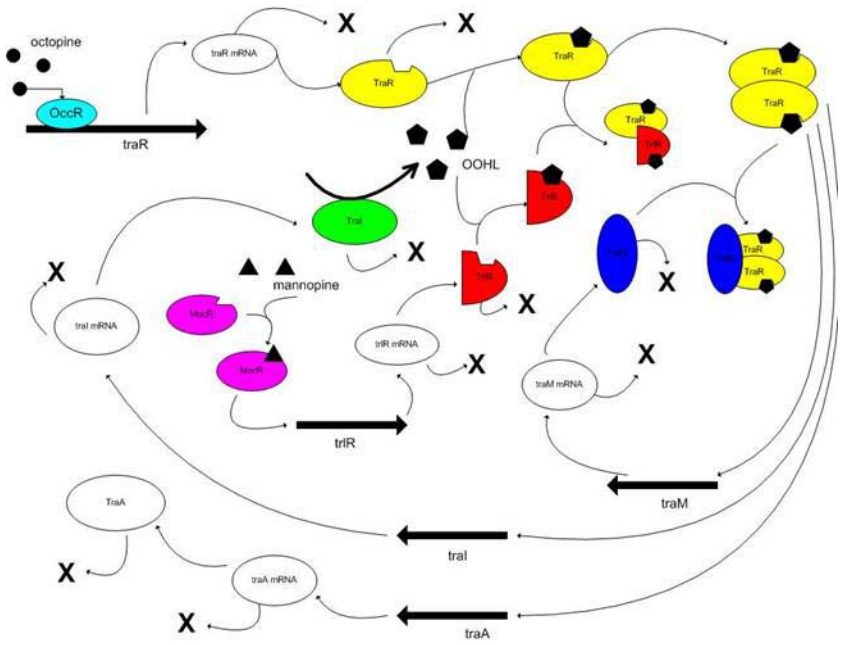

Figure 2. DMR-0218475. Statistical mechanics can be used to understand fitting of reaction rates in complicated biological processes, such as the one shown.

- All levels of funding mechanisms should be utilized to best advance cyberscience under DMR. These should include
  - Single investigator grants are the best mechanism for ensuring innovative advances in science, algorithms and software. They also provide the greatest opportunities for revolutionary advances in materials research. The NSF should support additional mechanisms to make advances available to the community.
  - Grants for both small and larger interdisciplinary research groups, particularly groups comprised of some subset of physical scientists, mathematicians, statisticians, computer scientists, and engineers are needed. Some of these grants should be in the funding range of one to two million dollars per year.
  - Grants for large centers to serve the computational and education needs of the broader materials research theory community are needed.
  - We recommend having a targeted software infrastructure solicitation to bring hardware and software advances to a broader community. The mechanism to bring well-developed codes to a wider audience has not worked in the past. Supported activities should include documentation, user training, and maintenance of community codes. We recommend that a standing panel of experts select the software related activities proposed by small or large groups based on anticipated 5 year impact, user surveys, technical merit and expertise of the proposers.

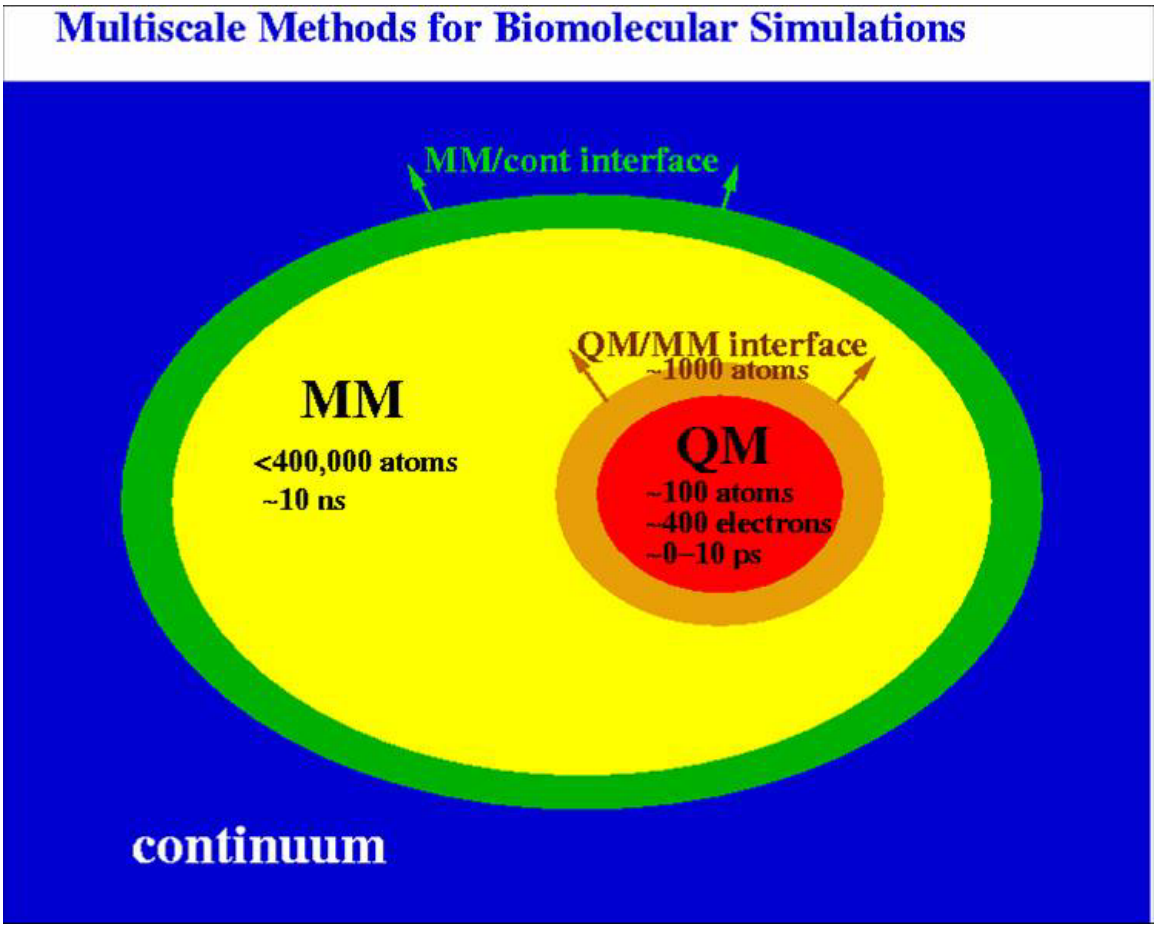

Figure 3. DMR-0121361. This figure illustrates multiscale modeling for materials, including biomolecular simulations, showing the interfaces between various computational methodologies. The practical limits on the number of atoms and the time scales that can be performed in calculations are outlined.

- Education and development of human resources within cyberscience should be addressed by NSF.
  - Adequate funding for undergraduate and graduate students in materials research cyberscience.
  - Hands-on workshops should be funded to disseminate new developments and encourage entry into new fields. This should support participation at all levels including graduate students, post-docs, young researchers and established scientists moving into new fields.
  - Programs that allow interdisciplinary groups to form and interact on an ongoing basis should be funded.
  - The possibility of web-delivered colloquia, workshop presentations, and even graduate-level specialty courses via distance learning should be explored.
  - Software geared for ease of use in classes that span materials research areas should be developed and made available for the general public and the materials research community.
- DMR should consider dedicating some resources specifically for research on materials for cyberinfrastructure: including both research for revolutionary advances

in computing, and research into projects that may contribute to the Moore's law-like growth of cyberinfrastructure. Such projects may include cyberscience applied to materials that may be used in cyberinfrastructure or design of algorithms to better model the behavior of devices that are applicable to cyberinfrastructure. The goal is to use cyberscience to improve cyberinfrastructure which will enable further increases in cyberscience.

- DMR should further evaluate how cyberinfrastructure can impact the cyberscience that can be performed within DMR. In particular, this report only concentrates on the cyberscience within DMR theory program. DMR should consider the broader issues of how to integrate the materials research theory program cyberscience requirements with those of the other DMR programs, and with other programs within MPS and the NSF.

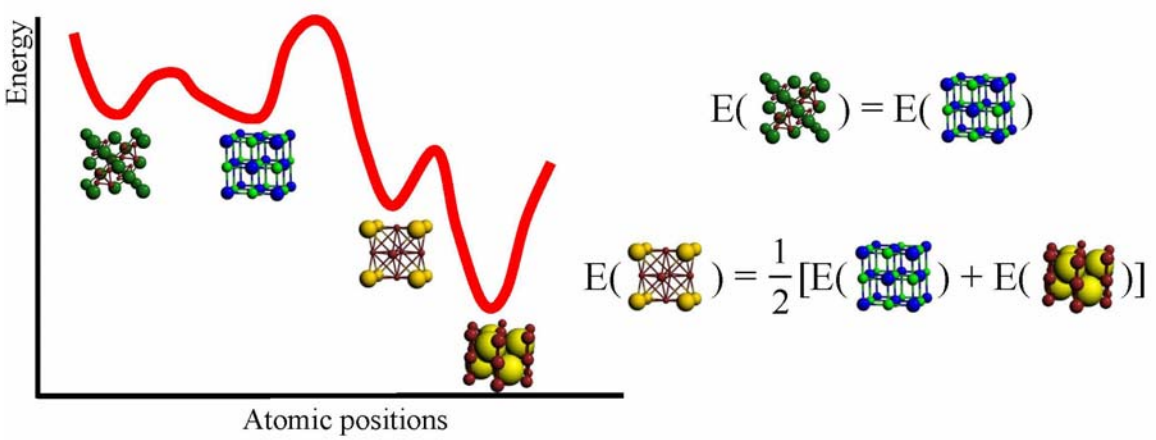

Figure 4. DMR-0312527. This illustrates the use of data mining to search for materials with novel properties.

Executive Summary --- Review of current activities

The current research performed under ITR grants administered by DMR in the Mathematical & Physical Sciences (MPS) directorate, is diverse, reflecting the diversity in the theory of fundamental phenomena in materials, materials synthesis and processing, structure and composition, properties and performance, condensed matter physics, and materials education. Under cross-cutting projects were solutions of large-scale eigenvalue problems for quantum systems, studies of extremal optimization, and using non-equilibrium surface science and network methodologies to study and implement parallelization in a broad class of algorithms called discrete event simulations. Presentations under electronic structure included new algorithms and codes using current density functional theory in magnetic systems and dynamical mean field theory for electronic properties and lattice dynamics in strongly correlated systems. Computational materials studies to guide experimentalists in synthesizing materials with novel properties for various engineering applications involved algorithms for multiscale methods, data mining, and high throughput first-principles methods. Presentations on computational mechanics included multiscale simulations of plastic flow and stress, with relevant information passed from one length scale to the next, and large scale dynamical simulations of hardening and nanoindentation. Presentations on computational materials for nanoscale science and engineering included studies of spintronics, wing crack dynamics, silicon quantum nanowires, tunneling in carbon nanotubes, and current-voltage characteristics of molecular electronic devices. A number of studies important for quantum computers and materials for next-generation cyberinfrastructure were presented. Presentations on strongly correlated systems included algorithm advances and applications to study materials ranging from liquid helium to high-temperature superconductors. The interface with biological systems and polymers included use of first-principles calculations for biological systems, application of statistical mechanics ideas to study protein design, ordering on curved surfaces, and models for understanding experimental results on biological pathways. Appendix A lists further details of the June 2004 review.

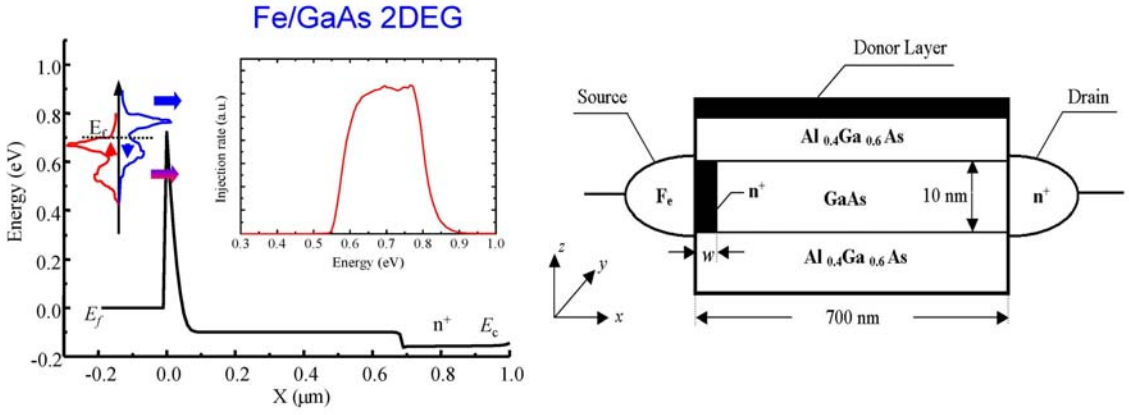

Figure 5. DMR-0121146. This illustrates the modeling a heterostructure device for spin injection with a Schottky source contact.

Almost all of the presentations showcased the algorithms and software developed to answer the important physical questions, as well as the applications to physical systems.

Summary of discussion concerning recommendations of cyberinfrastructure for NSF MPS DMR

For this report, cyberscience refers specifically to the science that can be accomplished within the materials theory program of DMR in its support of the wide range of programs addressing fundamental phenomena in materials, materials synthesis and processing, structure and composition, properties and performance, condensed matter physics, and materials education. Cyberinfrastructure refers to the algorithms, models, software, networks, and hardware that are required to perform the cyberscience investigations of materials theory. The educational needs for the next generation of researchers to be able to perform cyberscience with cyberinfrastructure will also be addressed. What is meant by cyberscience within the MPS directorate of NSF is much broader than is considered within this report. Furthermore, the recommended cyberinfrastructure and funding mechanisms proposed here may not be appropriate for all divisions within MPS. In particular, since DMR supports a wide range of programs addressing fundamental phenomena in materials, materials synthesis and processing, structure and composition, properties and performance, condensed matter physics, and materials education, not all of these programs would benefit to the same degree with advances of any one aspect of cyberinfrastructure. It is assumed that at least the current amount of cyberinfrastructure available to materials researchers through the NSF will grow. For example, both the PACI (National Partnership for Advanced Computational Infrastructure) or the follow-on program CORE (Cyberinfrastructure Open Research Environment) resources and monies for small individual researcher computers and clusters should continue to be available for members of the materials research community. Because of the unique needs of the materials research community, some of the recommendations within this report may not agree with recommendations of other NSF-sponsored reviews of cyberscience and cyberinfrastructure. There are other programs, and indeed other divisions, within MPS where there is nearly a single cyberinfrastructure bottleneck to further advances in their particular cyberscience. No such single cyberinfrastructure bottleneck exits for materials theory, rather there are multiple cyberinfrastructure bottlenecks that need to be overcome to further the cyberscience within the materials research theory program.

Appendix B contains summaries of the responses, together with the questions, of the questionnaire concerning materials research theory issues in cyberscience and cyberinfrastructure. These questions were jointly developed by some of the authors of this report together with the DMR theory program directors. The questionnaire was distributed at the June 2004 review, and participants either filled in a paper copy or sent in their responses electronically. During the June 2004 review all of Saturday morning was devoted to short presentations and free-ranging discussions of cyberscience and cyberinfrastructure. The outcomes of these discussions are also included within this summary of recommendations.

The recommendations by the Review participants for the cyberinfrastructure needed for cyberscience within the DMR theory program included:

❖ Continued advances in materials theory requires that the MPS directorate take the lead in providing the advanced cyberinfrastructure needed for materials theory.

Predictions of the properties of materials are a key problem: future advances in many fields are dependant on it. Design of materials is certain to become a major engineering field with important implications at the level of the national economy. Examples may include design of materials with simultaneously the desired strength, electrical transport properties, and magnetic properties. However, a major bottleneck at the present time is cyberinfrastructure: computational design of materials will place many orders of magnitude greater demands on algorithms, software and hardware performance. Nanomaterials is another important area: as devices get smaller, atomic level theory becomes both easier and more important. Examples include carbon nanotubes with their strength and electrical properties and nanoscale magnets that have self-assembly properties. There should remain research focused on understanding complex materials, such as those giving rise to magnetism and superconductivity. There has been steady progress in this field. It is likely that in five years the confidence in the computational results will go from moderate to high as the techniques advance. As a result, simulations of these materials will become routine. We cannot anticipate the many other areas that may need funding.

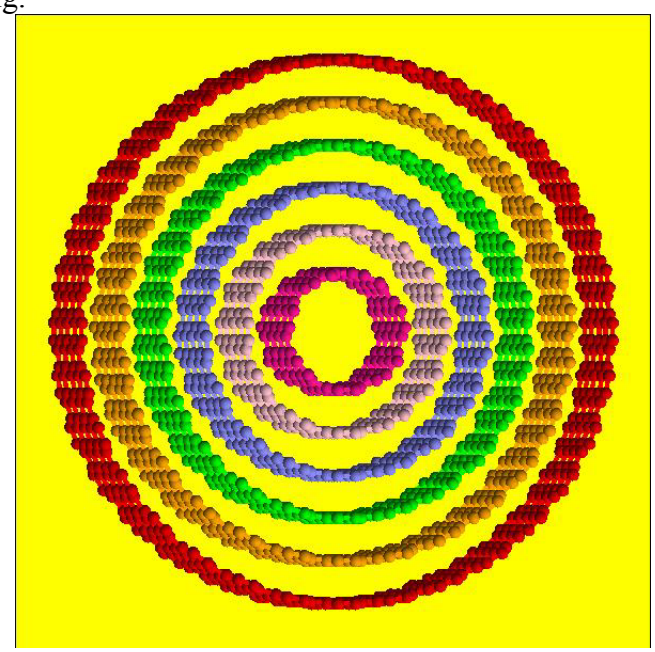

Figure 6. DMR-0112824. This is a view looking into a multiwalled carbon nanotube.

There needs to be a basic computational materials theory component to cyberinfrastructure: The continued development of both computational density functional theory and many body calculations connect strongly to cyberinfrastructure both by using its resources and contributing to its development. Both these fields have a rich past, but also an important future. There are continual breakthroughs which are pushing computational materials theory forward. For example in the area of correlated quantum systems, the last five years has seen the development of loop algorithms and the stochastic series expansion so that quantum spin simulations can be done on lattices 1-2 orders of magnitude larger. There has also been the integration of DFT with many-body

methods such as in the "LDA+DMFT" approach. Though such advances are typically made with individual PI grants, funding of larger interdisciplinary groups needs to be provided to capitalize on these and other advances.

There are different scales of cyberinfrastructure within DMR required to perform materials theory. In particular, some cyberinfrastructure is unique to the materials research community and some is small scale. Other required materials theory cyberinfrastructure has possible commonalities with the cyberinfrastructure in other divisions of MPS. DMR should explore coordinating shared cyberinfrastructure with other divisions in MPS when such coordination will most cost effectively advance cyberinfrastructure for DMR and other divisions in MPS. Many different shared cyberinfrastructure resources are envisioned to be needed to advance materials theory. There is not a single cyberinfrastructure bottleneck within materials theory. Another NSF division could take the lead if they have a single major cyberinfrastructure bottleneck, thereby freeing up DMR resources to tackle other materials theory cyberinfrastructure bottlenecks. For example, some MPS divisions have cyberinfrastructure bottlenecks for problems that are 'data intensive' and 'data analysis driven'; such as projects in observational astronomy, high energy experimental physics, and experimental nuclear physics. Although there are some data-intensive projects in materials theory, any cyberinfrastructure solution to the data-intensive problem that the astronomy/high-energy/nuclear communities advance may work for materials theory data-intensive problems. In other words, DMR theory should piggy-back off other parts of NSF to overcome cyberinfrastructure bottlenecks whenever possible in order to overcome materials theory cyberinfrastructure bottlenecks. This should allow DMR theory to concentrate more resources on other cyberinfrastructure bottlenecks for materials theory.

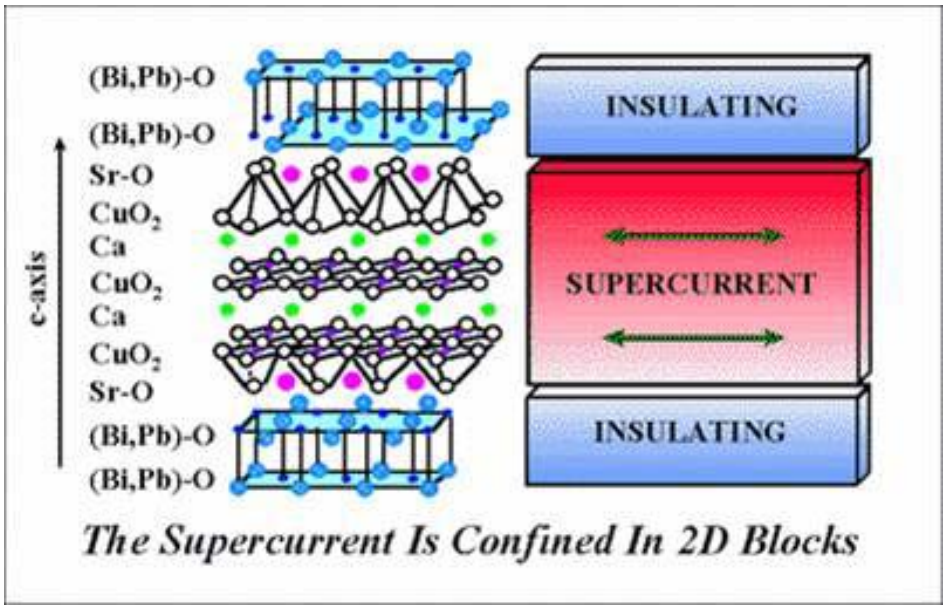

Figure 7. DMR-0314228. This illustrates that the function of a material follows from its structure.

- All aspects of cyberinfrastructure are important to perform cyberscience in materials theory. In contrast to other areas of scientific research, no one computer methodology or cyberinfrastructure bottleneck exists in this diverse community.
  - Algorithmic and software advances are equally important to equipment advances, and should be funded in proportion to its importance in cyberscience.
  - Development of new efficient computational methods must be recognized as a crucial scientific activity that will lead to future scientific advances in the same way that experimental techniques can open up new fields of scientific research.
  - NSF should realize that much of the funding is for human resources, with the timelines and needs different from the equipment portion of cyberinfrastructure. The growth rate of cyberinfrastructure, including both hardware and networks, can be viewed as improving smoothly with time in a Moore's law-like fashion. However, algorithmic advances and model advances tend to be much more revolutionary than evolutionary. Revolutionary advances are difficult to predict, while evolutionary advances are easy to predict. Consequently, many small projects to fund research in models and algorithms are probably the best way to guarantee that revolutionary advances do occur. The best of these revolutionary advances need a different funding mechanism to bring them to complete fruition. The funding needs for software development, as detailed below, are again different from those for algorithms, models, or hardware.
  - Access to compute power at all levels is needed to advance materials research applications: single workstations, small networked clusters and cycles on state-of-the-art supercomputers. The latter is a 'time machine' that can allow researchers to develop software and algorithms that will come into widespread use as computational resources grow. Computer centers are also needed to provide resources unavailable to university based researchers. In particular, there is a need to continue and expand current computer center resources for the materials research community, such as the PACI (Partnership for Advanced Computational Infrastructure) resources or the follow-on CORE (Cyberinfrastructure Open Research Environment).
  - Access to reliable high-bandwidth networks is important to many in the materials research community, particularly those not at major research universities.

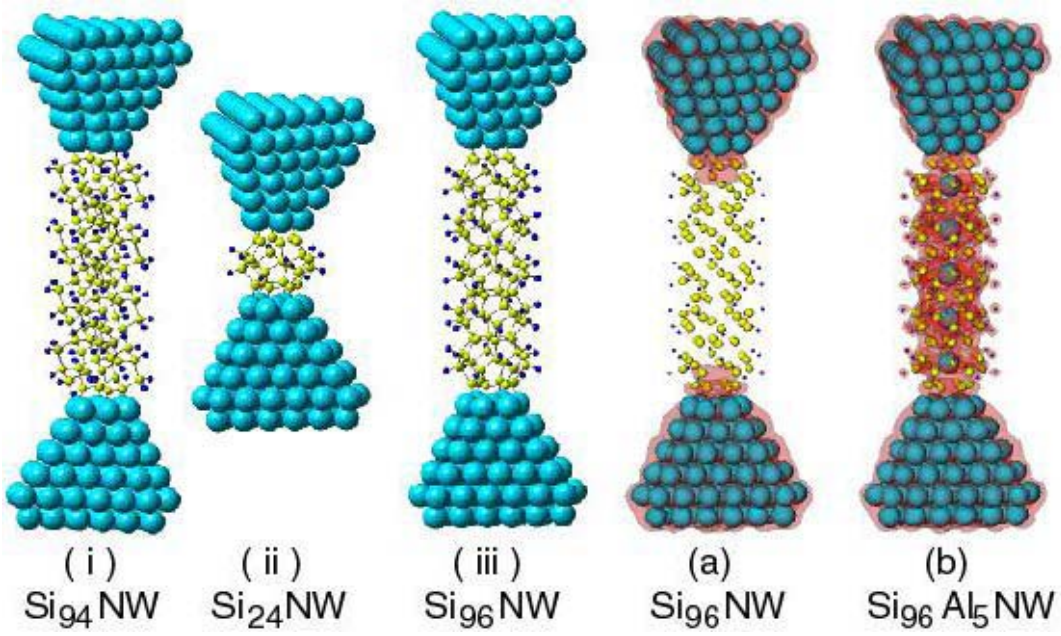

Figure 8. DMR-0205328. Various nanomaterials that form nano-wires (NW) between metal electrical contacts are shown.

- All levels of funding mechanisms should be utilized to best advance cyberscience under DMR. These should include:
  - Single investigator grants. This is the best mechanism for ensuring innovative advances in science, algorithms and software. This is the stage of research where there is the greatest opportunity for creation of new algorithms that will revolutionize materials theory and applications. This is also where the majority of educational opportunities exist for training the next generation of researchers for cyberscience. There exists a need for additional support to make such advances available to the community and a need for the development of a culture of shared, tested software.
  - Grants to groups (small or large) that will improve and maintain the most successful codes for use by the community. This can be a special grant or part of the grants mentioned below, but in any case it should be explicitly identified in the activity.
  - Grants for both small and larger interdisciplinary research groups, particularly groups comprised of some subset of mathematicians, statisticians, computer scientists, physical scientists, and engineers. Some of these grants need to be in the funding range of one to two million dollars per year since this is a represents an effective size for group interactions.
  - Grants for large centers to serve the computational and education needs of the broader materials research community.
  - Grants for software infrastructure. Software infrastructure is important to support the needs of segments of materials researchers, but falls outside normal grant timeframes and traditional grant deliverables and often fails to be funded. Multiscale research and materials design, in particular, will create a great need for software, beyond the resources of a typical university research group to develop. We do not expect that commercial vendors will provide the open-source, research

level codes that are needed in the materials research community. A distinct software funding mechanism is needed to support the development, maintenance, and user training of codes needed by the materials research community. We recommend that a standing panel of "experts" rank the software proposals based on specialized criteria. The goal of the panel should be to promote the use of the software in the materials research community. Appropriate selection criteria include user surveys, past experience of the institution in software development, utility of the software within the community, efficiency, reliability and user-friendliness of the software and so forth.

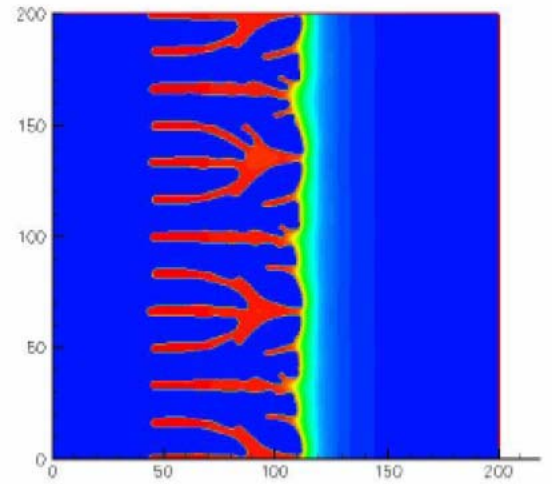

Figure 9. DMR-0121695. Non-equilibrium surface growth for microstuctures calculated using multiscale modeling.

- DMR should consider dedicating some resources to research on materials for cyberinfrastructure including both research for revolutionary advances in computing and research into materials that may contribute to the Moore's law-like growth of cyberinfrastructure. Although Moore's law for the growth of the central processor unit speed, and associated reduction in size of the integrated circuits, is well known, other parts of cyberinfrastructure have additional Moore's law-like growth. One example is the Moore's law-like growth in magnetic recording used in hard drives, with the associated reduction in size of the area used to write a single bit of data. Another example is the Moore's law-like growth of the speed and capacity of computer networks.
  - DMR is in a unique position to encourage research that may be relevant to future cyberinfrastructure.
    - DMR should encourage materials studies and condensed matter physics studies that may be relevant to revolutionary changes in cyberinfrastructure. One past example would be the change from tube technology to transistor technology and integrated circuits in computers due to advances in semiconductors and surface science. Another example is the recent revolutionary change in magnetic recording read head technology that was ushered in with the discovery of materials that have the property of giant magnetoresistance. Perhaps in the future quantum computing, biological computing, or other technologies may revolutionize cyberinfrastructure.

Other revolutionary material advances may find new classes of materials that have dual properties that usually are mutually exclusive, such as materials that might simultaneously have both a magnetic moment and an electric polarization --- a material which could revolutionize data storage technologies.

- DMR should encourage materials studies that may be relevant to future evolutionary changes in cyberinfrastructure that could continue Moore's law-like advances in cyberinfrastructure. In particular, this research may address materials issues that may present obstacles to Moore's law-like growth due to physical limitations. One example is the lack of thermal stability in modern magnetic recording technologies, due to smaller grain sizes (called the superparamagentic limit) and larger recording densities. Another is recent progress to overcome interconnect failure due to electromigration of atoms. Both of these are only currently becoming problems because the length scales of the devices are approaching the fundamental lower length scale for materials: the atomic length scale.

- This research may be both in the areas of the science of materials, and for less materials-oriented research, for example into research of vulnerability and reliability and scalability of cyberinfrastructure. Some of this type of research is in materials theory in the broad sense, including statistical mechanics (both equilibrium and non-equilibrium), interacting agents, network theory, random-matrix theory, and catastrophe theory.
- This research should not necessarily be geared toward the next generation of cyberinfrastructure, but to cyberinfrastructure in a five to fifty year time frame.
- The research within DMR theory will increasingly blur the boundary between materials structure and function, as well as the boundary between materials and devices. This is because as cybertechnolgy continues to advance and approach atomic dimensions quantum effects become increasingly important. One current example of this blurring is demonstrated by the active area of research into molecular electronics.

- DMR should further evaluate how cyberinfrastructure can impact the cyberscience that can be performed within materials research. In particular, this report only concentrates on the cyberscience within the DMR theory program. DMR should consider the broader issues of how to integrate the materials research theory program cyberscience requirements with those of the other DMR programs, and with other programs within MPS and the NSF.
  - Although the June 2004 review focused on the materials theory program within DMR, the availability of cyberinfrastructure and its ability to facilitate cyberscience extends to the other programs within DMR. DMR should not have a narrow view of cyberscience and cyberinfrastructure.
  - Much of the cyberscience within the materials theory program is cross-disciplinary or multidisciplinary. It is recommended that funding mechanisms that enhance and encourage such research continue, which requires that the DMR theory program coordinate with other programs within DMR, with other divisions within MPS, and with other directorates within NSF.

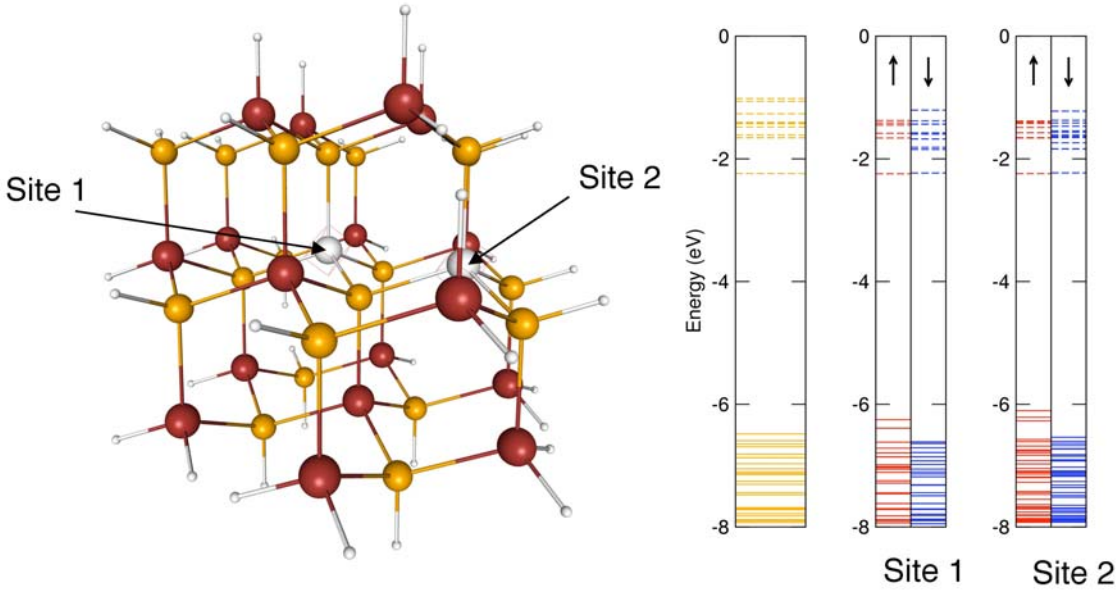

Figure 10. DMR-0325218 Energy bands for $MnZn_{18}Se_{19}$ quantum dots are shown.

- NSF should consider new methods of enhancing cyberinfrastructure for the materials research community.
  - The existence and growth of the PACI or CORE program (or something like them) to provide cyberinfrastructure resources for materials researchers is a crucial component of enabling cyberscience.
  - One possibility to consider would be to have a materials science grid of available computers to help satisfy the computing needs of DMR researchers. Sufficient funding would have to be available on an on-going basis in order for this computing grid to be productive for the materials research community at large. Such a computer grid may include traditional supercomputers, clusters, and loosely-organized computers within the 'SETI-at-home' model of computing. Such a loosely-organized mode of computing may only satisfy the fraction of materials researchers who have many decoupled computational tasks.
  - A central repository for important computational materials results, similar to protein data banks. It should be investigated whether this could be done with the appropriate archival journals.
  - A software repository for materials algorithms and for materials software. To be efficient, support for only one such repository should be funded.
  - An education software repository for simulations for the enhancement of education in materials at all levels, from K-12 to advanced graduate courses. This repository should also contain definitions and explanations of the specialized jargon that is common in the cyberscience studies of materials. To be efficient, funding for only one such repository should be funded.
- Education and development of human resources within cyberscience should be addressed by NSF. Lack of training results in a many year lag between the development of techniques and their use within the community with a consequence of wasted human resources and hardware. There is a very uneven level of technical expertise across institutions and fields. An ongoing, interdisciplinary series of

workshops and other training will help keep the academic community at the leading edge.

- Adequate funding for researchers, including undergraduate and graduate students, in materials research cyberscience is needed.
- Hands-on workshops or schools for researchers should be funded. Examples of workshops include those on algorithms, software development tools, training on important codes, and methods. These workshops should be aimed primarily to graduate students and junior post-doctoral researchers.
- The possibility of web-delivered colloquia, workshop presentations, and graduate-level specialty courses via distance learning should be explored. This will not duplicate what exists at typical universities, but instead focus on specialized topics. Expertise and facilities at the Supercomputer centers, for example, could be enlisted for this effort.
- Software geared for ease of use in classes that span materials research areas should be developed and made available for the general public and the materials research community.

The possibility of breakthroughs in materials research theory that could be enabled by adequate cyberinfrastructure is very exciting. The possibilities in theory that are dreams today may become realities. However, only some of these dreams can be described here. Furthermore, it is entirely possible that advances in cyberinfrastructure will create revolutionary advances that are not on anyone's 'radar screen' today. That is one of the joys of research. Materials research theory dreams that may become reality include:

- Designing nanoscale structures with desirable functional properties to be used as components in nanoscale electronics and nanoscale optoelectronics.
- To realize the potential of using nanostructures in device applications.
- To enable large-scale fabrication of nanostructures with desired structural and functional properties.
- Predictive analysis of the growth of nanostructures, and the dynamics and failure modes of nanodevices and nanostructures.
- Algorithms that exploit distributive computing to circumvent the limitation on the accessible simulation time in simulations of dynamics of materials and devices.
- The predictive behavior of materials composed of the marriage of bio-molecules (proteins, enzymes, DNA), electronic components, optoelectronic components, chemical nano-factories, and non-biological materials (nanotubes, polymers, etc.)
- Using ideas of statistical mechanics to provide predictive and user-friendly scalable algorithms for cyberscience and for industrial, homeland security, and military applications.

Such advances in materials lead to advances in technology which can be used to improve the life of the peoples and the environment of the world.

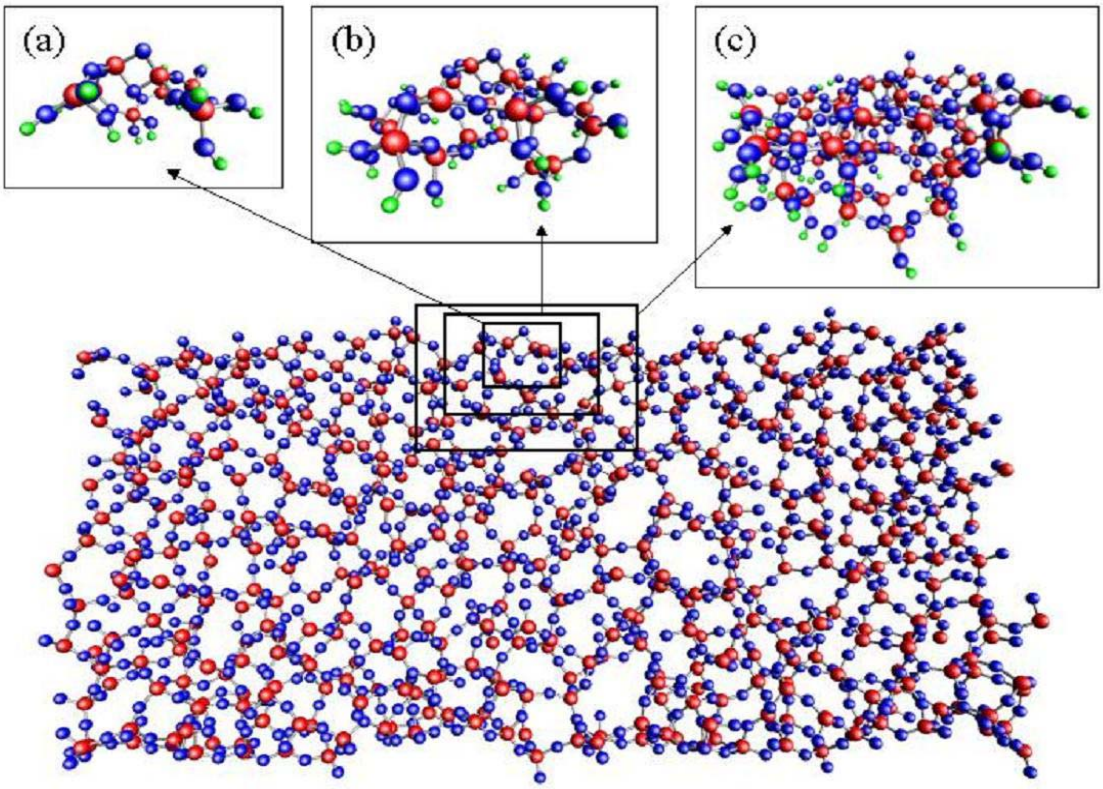

Figure 11. DMR-0325553. An amorphous silicon surface shows that portions of the surface correspond to a particular atomic arrangement.

APPENDIX A: NSF ITR Computational Science Review

June 17—19 the 2004 NSF Computational Materials Science Review was held at the Materials Computation Center at the University of Illinois Urbana-Champaign. Invited presenters included all principle investigators, as well as other senior personnel, post-doctoral fellows, and graduate students involved in DMR ITR awards. In total, 110 researchers were registered participants, including 44 PIs and co-PIs, 35 graduate students, and 22 post-doctoral fellows. The first two days consisted of presentations and posters of the research performed under the NSF Division of Materials Research (DMR) Theory and Information Technology Research (ITR) grants. The talks were broken up into the broad categories individually described below: crosscutting, electronic structure, computational materials, computation mechanics, computational materials on the nanoscale, quantum coherence control and quantum information systems, correlated systems, polymers, and the interface with biology. Further information can be found at http://www.mcc.uiuc.edu/NSFitr04rev.

The current research performed under ITR grants administered by DMR in the Mathematical & Physical Sciences (MPS) directorate, is very diverse. This reflects the diversity in the area of fundamental phenomena in materials, materials synthesis and processing, structure and composition, properties and performance, condensed matter physics, and materials education. Specific interesting advances and explicit cyberinfrastructure needs are listed under the general subtopics below. These are organized in the order of presentation at the conference. The complete schedule is listed at the end of this appendix.

Crosscutting:
Under cross-cutting projects were solutions of large-scale eigenvalue problems for quantum systems, studies of extremal optimization, and using non-equilibrium surface science and network methodologies to study and implement parallelization in a broad class of algorithms called discrete event simulations.

Electronic Structure:
Presentations under electronic structure included the development of object oriented codes for general electronic structure calculations, GUI interfaces created for high school students to carry out realistic electronic calculations, research on functionals for magnetic systems, investigations of electronic response in time dependent density functional theory (TDDFT), and the maturation of dynamical mean field theory (DMFT) into a practical approach for realistic calculations of electronic properties and lattice dynamics in strongly correlated systems. The latter is an extension of the density functional approach to "spectral density functionals" which has led, for example, to the first successful quantitative theory able to describe the famous anomalous behavior of Pu.

Computation Materials:

Computational materials activities aimed to guide experimentalists in synthesizing materials with novel properties for various engineering applications were reported. They involved algorithms for data mining, multiscale methods, transferable semi-empirical Hamiltonians (including self-consistency and multi-center interactions) and high throughput first-principles methods. Research presented varied from theoretical prediction of entirely new classes of materials and phenomena, such as "multiferroics" that couple ferromagnetic and ferroelectric behavior, to large scale computational optimization of materials for important applications, using data mining and efficient *ab initio* calculations. In addition, new algorithms were presented for thermodynamic correlations of density/composition waves and time-dependent behavior, such as non-linear crack development and propagation, using finite elements in space and time.

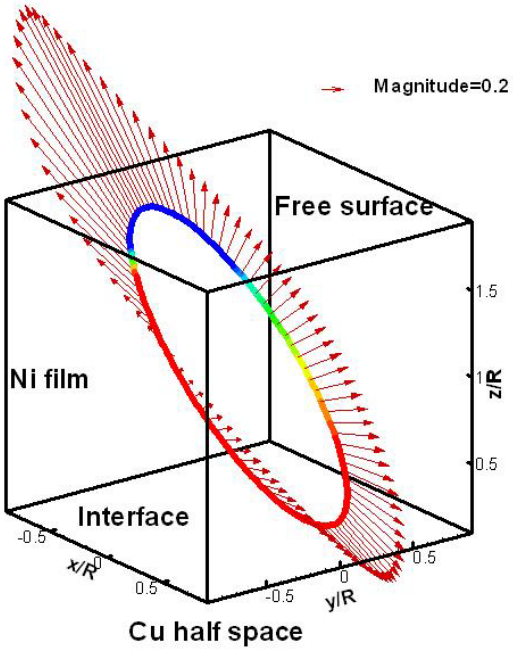

Figure 12. DMR-0113555. The stress field of dislocation loops in a thin film of copper and nickel are sketched.

Computation Mechanics:

Presentations on computational mechanics included multiscale simulations of plastic flow and stress, with research into optimal ways to pass the relevant information from one length scale to the next, and large scale simulation of strain hardening that demonstrates surprising effects due to elastic anisotropy that is very difficult to include in analytic models. The emergence of multiscale modeling is bringing together the field of large scale mechanics with materials computation of dynamics at the nano and atomic scales.

Computational Materials at the Nanoscale:

Presentations on computational materials for nanoscale science and engineering included studies of spintronics, wing crack dynamics, silicon quantum nanowires, tunneling in carbon nanotubes, and current-voltage characteristics of molecular electronic devices.

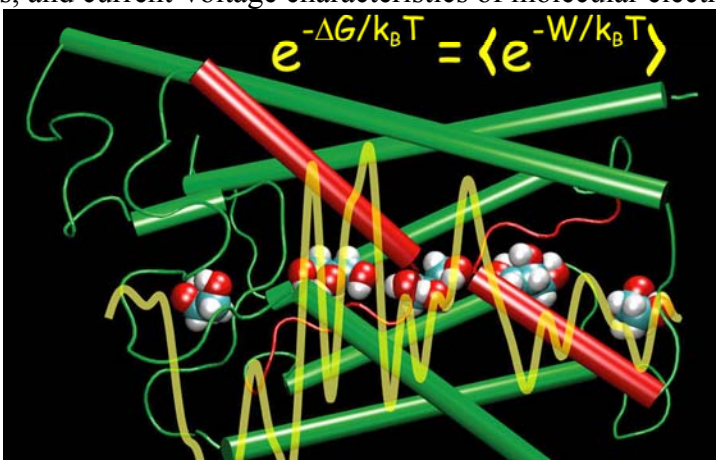

Figure 13. DMR-0325939. Symbolically demonstrates an algorithm to simulate thermodynamic structure and properties of proteins and biomolecules.

Quantum Coherence Control and Quantum Information Systems:
A number of studies important for quantum computers and materials for next-generation cyberinfrastructure were presented including studies of decoherence in quantum devices and control of spin interactions by optical means.

Correlated Systems:
Presentations on strongly correlated systems included algorithm advances and applications to study materials ranging from liquid helium, to high-temperature superconductors and systems whose magnetic properties depend on highly correlated electronic states. Several of the contributions focused on algorithms to allow study of quantum systems with many degrees of freedom.

Polymers:
The interface with biological systems and polymers included both use of first-principle calculations for complicated biological systems to use of statistical mechanics ideas to study protein design, ordering on curved surfaces, and models for understanding experimental results of experiments on biological pathways.

Interface with Biology:
The interface with biological systems and polymers included both use of first-principle calculations for complicated biological systems to use of statistical mechanics ideas to study protein design, ordering on curved surfaces, and 'sloppy models' for understanding experimental results on complex biological pathways.

Workshop Presentation Schedule

Thursday, June 17, 2004

8:00-8:15	**Welcome** Johnson, UIUC/MCC
8:30-9:00	**TR and Cyberscience/Cyberinfrastructure** Hess & Taggart, NSF

CROSSCUTTING

9:00-9:30	**Materials Computation Center** Johnson & Martin, UIUC
9:30-9:45	**Solution of Eigenvalue Problems for Multi-Scale Phenomena by Quantum Monte Carlo Methods** Nightingale, Rhode Island
9:45-10:00	**Large-Scale Applications and Theory of Extremal Optimization** Boettcher, Emory
10:00	**Morning break**
10:30-10:45	**Synchronization and Extreme Fluctuations on Networks, and Application to Scalable Parallel Discrete Event Simulations** Gyorgy Korniss (Rensselaer) and Mark Novotny (Mississippi State)
10:45-11:00	**Simulating Extended Time and Length Scales Using Parallel Kinetic Monte Carlo and Parallel Accelerated Dynamics** Amar, Toledo

ELECTRONIC STRUCTURE

11:15-11:30	**Large-Scale, Grid-Enabled Gaussian Orbital Implementation of Current Density and Spin Density Functional Theory for Ordered Systems** Trickey, Florida
11:30-11:45	**Time-dependent density-functional-theory investigations of electron-hole** Eguiluz, Tenn
11:45-12:00 pm	**Computational Design of Strongly Correlated Materials** Sergej Savrasov, New Jersey Institute of Technology and Gabriel Kotliar, Rutgers University

12:00-1:00 **Lunch**

CROSSCUTTING

Statistical Physics and Computational Complexity (Poster)
Bowick, Marchetti & Middleton, Syracuse

1:00-2:30 **Poster session**
Poster presenters

Computer science and scaleable parallel methods for materials modeling (Poster)
Todd Martinez, Eric de Sturler

1:00-2:30 **Large-Scale Applications and Theory of Extremal Optimization** (Poster)
Stefan Boettcher

Multiscale Modeling Methods for Materials Science
P. Bellon, D.D. Johnson, D.E. Goldberg, T.J. Martinez, K. Dahmen, A. Hubler, and E. Luijten; Students: Kumara Sastry, Alexis L. Thompson, Jia Ye, Robert White, Glenn Foster, and Lei Guo

COMPUTATION MATERIALS

1:00-2:30 **Current DFT versus Ordinary DFT for Atomic Ground States in External Magnetic Fields**
(Poster)
Wuming Zhu, S. B. Trickey, and Ashley Alford II, Quantum Theory Project and Physics Department, University of Florida

CROSSCUTTING

Modelling disease outbreaks in realistic urban social networks
(Poster)
Hasan Guclu

ELECTRONIC STRUCTURE

Object-oriented Development of a Gaussian Basis DFT Code
(Poster)
J. Ashley Alford

CROSSCUTTING

Education Outreach and Knowledge-transfer (Poster)
Duane D. Johnson

ELECTRONIC STRUCTURE

Combining EDMFT with GW: Applications to Hubbard Model and Coulomb Ga (Poster)
Ping Sun and Gabriel Kotliar, Department of Physics, Rutgers University

CROSSCUTTING

Nanoscale Structures & Devices (Poster)
R. Martin

Stochastic Growth in a Small World and Applications to Scalable Parallel Discrete-Event Simulations (Poster)
H. Guclu, B. Kozma, G. Korniss, M.A. Novotny, Z. Toroczkai, M.B. Hastings, and P.A. Rikvold

Materials Simulation Toolkits (Poster)
J.N. Kim

COMPUTATION MATERIALS

2:30-3:00 **NSF ITR Project: MatCASE (Materials Computation and Simulation Environment)**
Liu, Chen, Du & Raghavan, Penn State

3:00-3:15 **High throughput *ab initio* computation and data mining for predictingmaterials properties**
Dane Morgan, MIT

3:15-3:30 **Computational design of novel multifunctional materials**
Spaldin, UCSB

3:30-4:00 **Multiscale models for microstructure evolution and response**
Haber, UIUC/CPSD

4:00-4:30 **Science and Software for Predictive Simulation of Chemo-Mechanical Phenomena in Real Materials**
Bartlett, Cheng & Trickey, Florida

4:30-4:45 **A Thermodynamic Density-Functional Theory of Static and Dynamic Correlations in Complex Solids**
Johnson, UIUC

4:45- **Afternoon break**

5:00

COMPUTATION MECHANICS

5:00-5:15 **Physics-Based Modeling of Plastic Flow that Couples Atomistics of Unit Processes with Macroscopic Simulations**
Bassani & Vitek, Penn

5:15-5:30 **Collaborative Research on Large-Scale Dislocation Dynamics Simulations for Computational Design of Semiconductor Thin Film Systems**
Ghoniem, UCLA

QUANTUM COHERENCE CONTROL AND QIS

Monte Carlo simulation of spin injection and coherent transport in a heterstructure device with a Schottky source contact (Poster)
Min Shen, Semion Saikin, Ming-C. Cheng, Vladimir Privman

5:30-7:00 **Poster Session/Discussion groups**

COMPUTATIONAL MATERIALS ON THE NANOSCALE

Electronic and optical properties of Ge nanowires (Poster)
A. Nduwimana, X.Q. Wang, L. Yang, X. Zhao, M. Y. Chou

QUANTUM COHERENCE CONTROL AND QIS

Optical control of exciton-polarons in organic semiconductors (Poster)
Michael Katkov

COMPUTATIONAL MATERIALS ON THE NANOSCALE

Vacancy Mediated Diffusion in Ni_3Al (Poster)
R. Tedstrom, M. S. Daw, C. Harris

Energetics of Silicon Nanostructures on the Si (Poster)
M. Yu, S.Y. Wu, and C.S. Jayanthi

QUANTUM COHERENCE CONTROL AND QIS

Electron spin decoherence due to interaction with nuclear spin bath (Poster)
Semion Saikin

COMPUTATIONAL MATERIALS ON THE NANOSCALE

The Transfer Hamiltonian: A Tool For Large Scale Molecular Dynamics Simulations Using Quantum Mechanical Forces (Poster)
DeCarlos E. Taylor, Keith Runge, Rodney J. Bartlett

Strain relaxation in epitaxial core-shell nanowire heterostructures (Poster)
R. N. Musin, X. Q. Wang

First-principles calculations of magnetic compounds and quantum dots (Poster)
Xiangyang Huang and Jim Chelikowsky

QUANTUM COHERENCE CONTROL AND QIS

Decoherence Rate of Semiconductor Charge Qubit (Poster)
Leonid Fedichkin and Arkady Fedorov

Friday, June 18, 2004

COMPUTATIONAL MATERIALS ON THE NANOSCALE

8:30-9:00 **Institute for the Theory of Advanced Materials in Information Technology**
Chelikowsky, Saad, Wentzcovich, Minnesota; Kaxiras, Harvard; Louie, UCB

9:00-9:30 **Modeling & Simulation of Quantum Phenomena in Semiconductor Structures of Reduced Dimension**
Chou, Landman, GIT, Umrigar, Cornell, & Wang, Clark-Atlanta

9:30-9:45 **Billion-Atom Multiscale Simulations of Nanosystems on a Grid**
Vashishta, Kalia & Nakano, USC

9:45-10:00 **A New Understanding of the Suppressed Tunneling Conductance in Multi-Wall Carbon Nanotubes**
Jayanthi & Wu, Louisville

10:00-10:15 **Simulations of Open Quantum Systems for Molecular Electronic Systems**
Roland & Sagui, NCSU

QUANTUM COHERENCE CONTROL AND QIS

10:15-10:45 **Evaluation of Decoherence for Quantum Control and Computing**
Vladimir Privman

10:45-11:00 **Optical control of spin-spin interaction in doped semiconductors**
Piermarocchi, Michigan State

11:00 **Morning break**

CORRELATED SYSTEMS

11:30-11:45 **Study of complex nanoclustered states in magnetic and superconducting materials**
Elbio Dagotto, Univ of Tenn, Knoxville

11:45-12:00 **Quantum Cluster Simulations of Lower Dimensional Systems**
Jarrell & Zhang, Cincinnati

12:00-12:15 **Quantum phase transitions in magnetic impurity problems**
Ingersent, Florida

12:15-12:30 **Recent Progress in linear scaling Quantum Monte Carlo Algorithms**
Scalettar & Bai, UCD

12:30 **Lunch**

COMPUTATION MATERIALS

Optimization of phase diagram construction (Poster)
Maria Emelianenko

1:30-3:00 **Poster Sessions**
Poster presenters

COMPUTATION MECHANICS

Dislocation dynamics in epitaxial thin films (Poster)
E. Tan and L. Sun

COMPUTATION MATERIALS

Passive random walkers and global maxima of evolving surfaces (Poster)
T. Dubreus, M.A. Novotny, and A. Kolakowska

Structure and properties Silica bulk, surface, and wires (Poster)
Cao-Chao, Lin-Lin Wang, Chun Zhang, Mao-Hua Du, and Hai-Ping Cheng

Analysis of an Iterative Perturbation Scheme for Solving Inhomogeneous Elasticity Problem (Poster)
Peng Yu

Computational Investigation of magnetism and piezoelectricity in wurtzite MnO (Poster)
Priya Gopal and Nicola Spaldin

Dynamical multiscale approach to bridging classical and quantum interatomic potentials for the simulation of failure in amorphous SiO2 (Poster)
P.A. Deymier and K. Oh

Modeling Solidification Microstructures (Poster)
J. A. Dantzig, B. Athreya, A. Chang, L. Kale, and K. Wang

COMPUTATIONAL MATERIALS ON THE NANOSCALE

Lattice Vibrations in Silicon Nanowires (Poster)
Li Yang, X.Y. Zhao and M.Y. Chou

COMPUTATION MATERIALS

Spacetime Discontinuous Galerkin Methods in Materials Modeling (Poster)
R. Haber

Ordering in multicomponent alloys: where do the atoms go and why? (Poster)
Subhradip Ghosh,Daniel DeRoberts, Dominic Biava, Nikolai Zarkevich, D.D. Johnson

Toward hydrolytic weakening and stress corrosion cracking (Poster)
Ting Zhu, Ju Li, Xi Lin, Sidney Yip

POLYMERS

3:00-3:15 **Development of Quantitative Coarse-Grained Simluation Models for Polyolefin Blends**
Kumar & Garde, RPI

3:15-3:30 **Development of a Simulation Tool to Model the Complex Dynamics in Reacting Monomer/Polymer Mixtures**
Balazs, Pittsburgh

INTERFACE WITH BIOLOGY

3:30- 4:00	**Minimalist models and connections with large simulations for protein assembly and DNA recognition** Yaakov (Koby) Levy, CTBP
4:00- 4:30	**Tools and Methods for Multiscale Biomolecular Simulation** Sagui, Pedersen, Board & Bernholc, NCSU
4:30	**Afternoon Break**
4:45- 5:00	**Statistical Mechanics of Sloppy Models: Bacterial Cell-Cell Communication** Sethna, Cornell [Josh Waterfall]
5:00- 5:15	**A Protocol for Computational Protein Design** Zeng, GWU, & Tang, NEC
5:15- 5:30	**Ordering on Curved Surfaces** Mark Bowick
5:30- 7:00	**Poster Session/Discussion groups** Poster presenters

CORRELATED SYSTEMS

Quantum Monte Carlo study of planar quantum dots in magnetic fields (Poster)
A. D. Guclu, C. J. Umrigar, and M. Y. Chou

COMPUTATIONAL MATERIALS ON THE NANOSCALE

ODCII-to-Egamma center interconversion in amorphous silica (Poster)
Manuel Alemany and James Chelikowsky

QUANTUM COHERENCE CONTROL AND QIS

Amplification and Relaxation of Electron Spin Polarization in Semiconductor Devices (Poster)
Yuriy V. Pershin

INTERFACE WITH BIOLOGY

Fast Accurate Evaluation of Protein Solvent Exposure (Poster)
Dr. Naigong Zhang

A Method for Consistent Embedding in QM/CM Simulations (Poster)
Aditi Mallik, Keith Runge, James W. Dufty

COMPUTATIONAL MATERIALS ON THE NANOSCALE

TDLDA and many-body Green's function methods in organic molecules and clusters (Poster)
M. Tiago and J. Chelikowsky

First-Principles Calculation of the Electronic Properties of Potassium-Covered Carbon Nanotubes (Poster)
Alexander Tchernatinsky

First-principles study of semiconductor nanowires: electronic and optical properties (Poster)
Xinyuan Zhao, C. M. Wei, Li Yang, and M. Y. Chou

COMPUTATION MATERIALS

Cobalt doping of a low-energy interface in TiO2 anatase (Poster)
Rebecca Janisch, Sibylle Gemming, Nicola Spaldin and MichaelSchreiber

Evolution of energetics of silica clusters and bulk from quantum calculations (Poster)
Yao He, Ying-Xia Wan, Mao-Hua Du and Hai-Ping Cheng

Multiscale Methods for Microstructure Simulation (Poster)
M. Bendsoe, J. Dantzig, R. Haber, D. Johnson, B. Kraczek, J. Norato, D. Tortorelli, C. Xia, et al

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Saturday, June 19, 2004

8:30-8:45	**Welcome and opening remarks** Tom Weber NSF/Division Director/Division of Materials Research
8:45-9:00	**From ITR to Cyberscience/Cyberinfrastructure: Where does the materials research computational community want to go?** D. Hess/ G. Taggart NSF/ Division of Materials Research/ Materials Theory
9:00-9:45	**Summary of science presented over the last two days of DMR/ITR CW&R: What is the science being done and what is on the horizon?** Panel Discussion: David Ceperley, UIUC, Moderator
9:45-10:35	**Summary of MPS CI/CS workshop -- a view across MPS** Mark Novotny (Mississippi State), Richard Martin (UIUC)
10:35	**Morning break**

10:50-12:00	**Discussion on Computational Science Opportunities: What Cyberinfrastructure does the Materials Research Community need?**
12:30-1:00 pm	**Closing Remarks**

APPENDIX B: Comments from the Questionnaire

1.A. *Describe briefly two highlights from the talks and posters on Thursday and Friday during the workshop that you found interesting and important. You may use one from presented work in which you were involved.*

Listed, in order of presentation at the workshop, are highlights mentioned on the surveys. Numbers in parenthesis are the number of responders citing this research. A feeling that all of the works presented were important was expressed, with which was considered best very strongly influenced by the field of research of the responder. Some responders only mentioned a particular talk, while others provided details about the talk and why it was rated so highly. The details below to question ***1.A.*** try to reflect both levels of response specificity. Comments that addressed particular talks are highlighted with bullets, while general comments on a group of talks are listed without bullets.

CROSSCUTTING

- Johnson and Martin (3). SONY Playstation for novel quantum chemistry computing.
- Boettcher (2). Extremal optimization algorithms.
- Korniss and Novotny (3). Dynamics and synchronization of algorithms on networks.

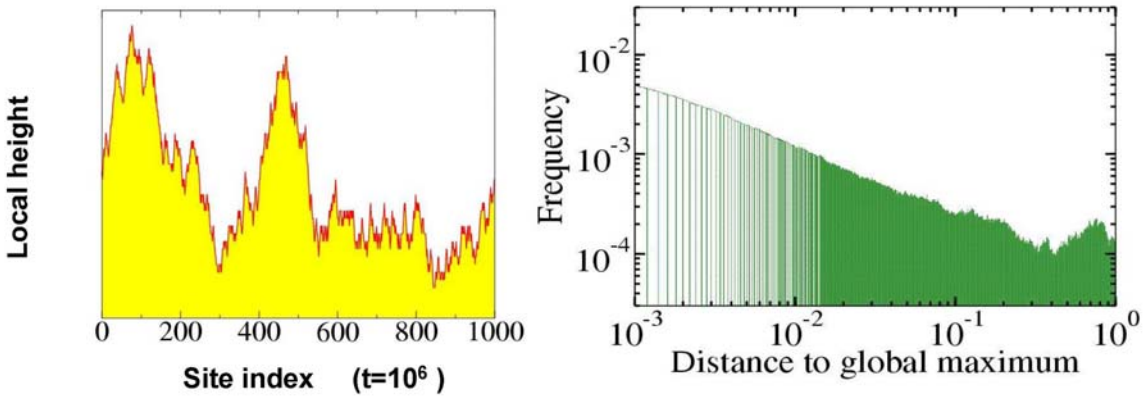

Figure 14. DMR-0113049. Non-equilibrium statistical mechanics, such as the surface (left) and properties of the surface (right) can be applied to obtain scalable algorithms for parallel computers.

ELECTRONIC STRUCTURE

- Trickey. Seriously working on exploiting grid physics infrastructure.
- Savrasov and Kotliar. The merging of dynamic mean field and LDA methodologies.

COMPUTATION MATERIALS

- Liu, Chen, Du, and Raghavan. MatCASE for Materials Computation and Simulation Environment.
- Morgan (3). First real example of non-trivial data mining in materials this responder had seen.

- Spaldin (3). Clever, not brute-force, approach to possible novel materials for evolutionary future cyberinfrastructure.
- Haber. Space-time multiscale finite-element methods.
- Bartlet, Cheng, and Trickey. Predictive first-principles algorithms.
- Johnson. Classical density functional theory based thermodynamics.

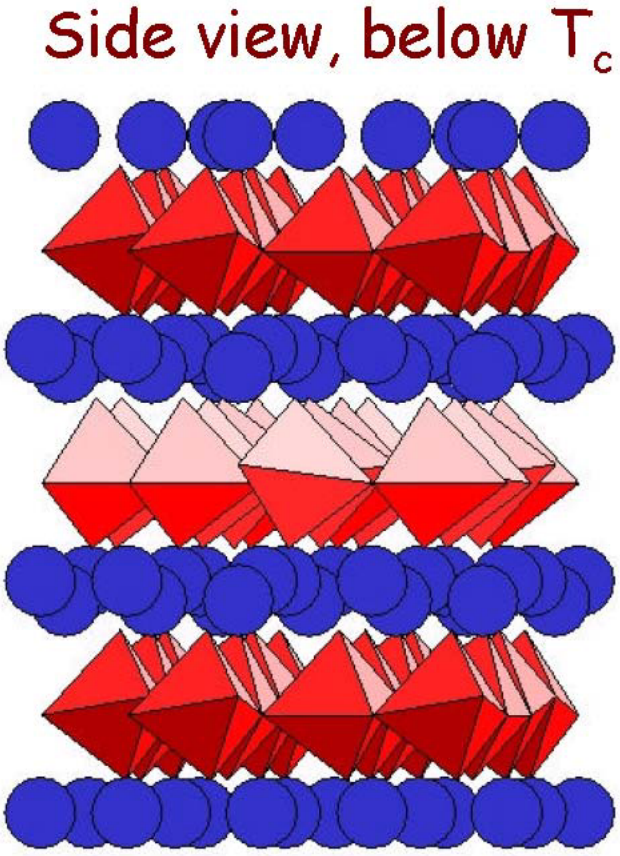

Figure 15. DMR-0312407. This shows a computational ferric material that has been designed from computer calculations.

COMPUTATION MECHANICS

- Ghoniem. Treatment of dislocation loops for a predictive theory of plasticity.

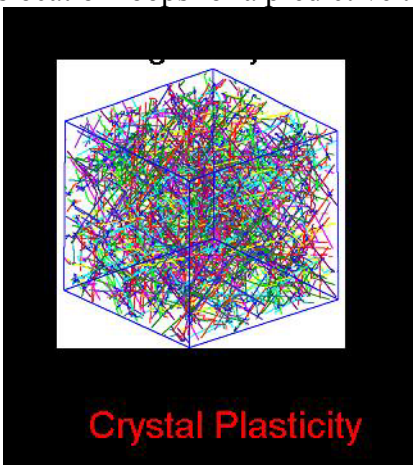

Figure 16. DMR-0219243. From a multi-slip model of crystal plasticity and dislocation dynamics, this shows dislocation lines.

COMPUTATIONAL MATERIALS ON THE NANOSCALE

There were no comments on specific talks, but one respondent stated that in their opinion the best talks were application or problem driven, specifically the Friday talks that were materials driven.

QUANTUM COHERENCE CONTROL AND QIS

- Privman. A systematic study of decoherence.
- Piermarocchi. The optical control of single spins and magnetization in semiconductors.

CORRELATED SYSTEMS

- Jarrell and Zhang. Intriguing comparative scaling presented for the algorithms.
- Ingersent. Exploring quantum phase transitions.

POLYMERS

Research at the border between polymers, nanomaterials, and biology was a highlight for one responder.

INTERFACE WITH BIOLOGY

Biologically oriented research was very interesting. Particularly interesting was the work at the nano-materials, biology interface.

- Sagui, Pedersen, Board, and Bernholc. Multiscale methods for more accurate biomolecular calculations.
- Bowick. Work on packing on curved surfaces.

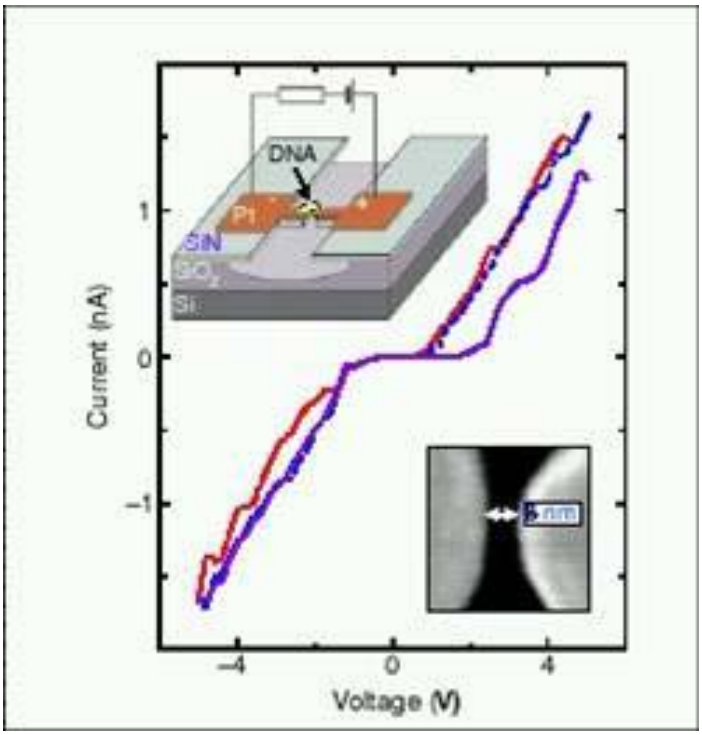

Figure 17. DMR-0312105. The electrical transport through DNA molecules is shown, including a picture of the experimental setup.

1.B. *Did the work in 1.A take advantage of any existing cyberinfrastructure? Could it have? If so, what?*

Since the presentations were funded from ITR awards, the universal consensus was that the talks in 1.A did take advantage of cyberinfrastructure.

This ranged from massively parallel supercomputers to individual compute clusters to workstations, with the underlying software and networks. It included algorithmic research on how to use the next generation of cyberinfrastructure, including grid computing, as well as how to efficiently utilize the machines available to the researchers. This also included work on multiscale GUI's for research by a number of groups. Other software utilized ranged from Mathematica to Globus.

1.C. *Can you imagine cyberinfrastructure that does not now exist (to your knowledge) within the materials research community that would have facilitated the scientific advances in 1.A or possibly even enabled even further progress?*

Cyberinfrastructure should support a more systematic web integration of the research efforts of various groups, including data and code sharing.

New cyberinfrastructure that does not now exist will include inventing, refining, and implementing new algorithms, and its associated mathematical underpinnings, to enable

research in cyberscience that could not be performed even with Moore's law progress in cyberinfrastructure.

DMR researchers need from cyberinfrastructure both good data bases and data mining. These may be started by individual researchers, but useful ones should then be accessible, standardized, and centralized. This could be aided by high-speed interconnects and accessible storage facilities.

The only remarkable hardware was the SONY Playstation machine, useful to see how computers of tomorrow can be developed and utilized.

Research would be enhanced by better access to machines. These would include supercomputers, large cluster-architecture machines --- not necessarily the fastest, but ones available on a daily basis, and small cluster-architecture machines.

The physicist's view of networks as dynamical systems provides a unique perspective to advance and understand the functioning of cyberinfrastructure.

A virtual reality coupling with experimental reality and real-time calculations, using a coupling between fast computers and sensors and actuators, could blur the boundaries between experiment, computations, and theory. (This possibility was heatedly discussed at the workshop.)

1.D. *Identify from talks or posters presented on Thursday and Friday during the workshop, any elements of cyberinfrastructure that were created (not including MCC) as a consequence of work supported under ITR.*

Algorithm advances to allow investigations of the science were present in many of the presentations and posters.

Several of the works included collaborations between various universities.

2. *What exciting future advances in computational materials research can be made with existing cyberinfrastructure? Feel free to discuss research areas within the broad umbrella of materials research (includes condensed matter physics, materials science, and solid state chemistry) that may not be represented at the workshop.*
A) on a 5 year time scale; B) on a 10 year time scale.

First – Essentially ALL advances today involve cyberinfrastructure. Communication is more and more an essential part of research at all levels. The most esoteric theoretical developments are often the ones most rapidly promulgated through the on-line archives. The increased utility of computation has brought together formally-disparate fields with cross fertilization through algorithmic features.

The present infrastructure is ALREADY greatly advanced over that of a few years ago.

(1) Algorithms have been and are more important than hardware (although both are important for progress). The ITR has been crucial in bringing experts together to reach the current level. Examples of algorithms developed or facilitiated by this combination:

Real space finite difference, finite-element, spline methods, wavelets, etc.
More efficient iterative diagonalization methods.
New techniques for "ab initio molecular dynamics"
New optimization methods, e.g., Genetic algorithms
Time dependent density functional theory and GW-Bethe saltpeter methods - optical properties
Quantum Monte Carlo methods
Algorithms for scalable codes on massively parallel computers
Multiscale algorithms to start to bridge the disparate length and time scales for materials
Better first principle methods, with greater accuracy and applicability

(2) The excitement is that computational materials research is now becoming a quantitative, rather than qualitative, predictive method. This is due to the cyberinfrastructure that is available, and further cyberinfrastructure will enhance the ability to guide synthesis and experiments in materials research.
In ten years, todays supercomputer calculations may be available on desktop computers. This will open up an entirely new area of research at the border between experiments and computations.

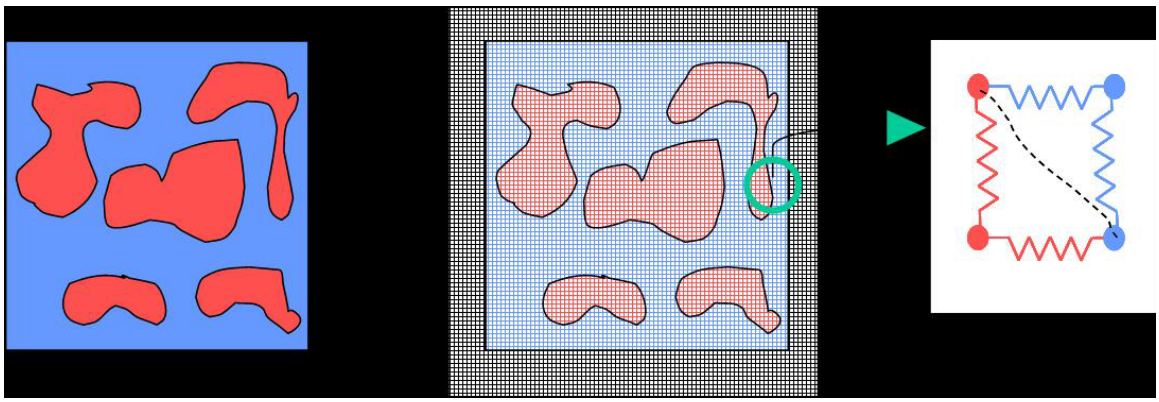

Figure 18. DMR-0312115. Multiscale modeling of microstructure can be applied to obtain processes such as coarsening within materials, with a portion of the interfacial region sketched in the right figure.

Overall Goals suggested for 5/10 year period:
(3) 5 years: First-principles search of new materials development through knowledgebase construction
10 years: Computational prediction of chemistry-microstructure-property relationships for complex, multicomponent systems Inverse materials design on a computer, i.e. materials property by design.

(4) 5 years: Effective coupling of atomistic and continuum models at device level
10 years: Same at the system level.

(5) 5 years: Development of electronic structure methods for correlated materials; practical methods for systems with large numbers of atoms (not strongly correlated)
10 years: Predictive capability for strongly correlated systems; Predictive capability for phase diagrams, crystal structures of large quantum systems

(6) 5 years: Accurate design of new materials with specific functionalities tailored for particular applications, in advance of their experimental synthesis.
10 years: Same as above, but for multiple functionalities in the same material

Explicit example of materials simulations that can be accomplished:
(7) 5 years: Complete description of microstructure evolution within one grain of a material during a typical life-cycle. This would include a reasonably complex alloy, following precipitation and phase evolution, then applying external loads and following the dislocation microstructure in full 3-D details.
10 years: Extensions to polycrystalline materials to include grain growth and grain boundaries.

(8) 5 years: molecular nanoelectronics, nano-bio-materials
10 years: Hi-Tc materials via first principles

Approaches for software to reach the goals:
(9) 5 years: The progress in the algorithms for materials simulation has been quite impressive. However, our community is slow in adapting new software engineering practices and utilizing the high-performance computing libraries, such as charm++, petsc for materials applications with few exceptions. Open source standards widely accepted for web applications (aka xml) can facilitate collaborations between groups and applications and integrations of multi-scale simulations. Open source tools made available by open source development (e.g., linux) and the project managements for code development.
10 years: Grid computing that will eliminate desktops. Dynamic code and test generations on-the-fly on a given architecture. Literate programming that can convert the algorithms to high-performance codes.

(10) 5 years: Central repository for important computational results – similar to protein data bank.
10 years: Linking such a data bank to multidisciplinary computer code, e.g., Quantum Chemical, Solid State, Biophysical, … to allow researchers to assemble multiscale simulations from a remote desktop. Simulations would run in a linked manner on multiple architectures.

Relation to individual investigator research and education:
(11) A lot of great science is being accomplished through the present US/NSF emphasis on funding single groups with their own individual computational approaches. This is in contrast with creation of widely used DFT codes, often from Europe. While lauding that accomplishment, we also need to ask the question: What basic individual science could have been done instead with those resources?

The second question is: How does the use of `black box' simulation codes affect graduate education? Do our students suffer by a lessening emphasis on writing their own programs? The experience of the DFT community could be assessed to decide on approaches to maintain the proper balance.

(12) (5 years) Enhanced predictive powers for accurate ground and excited properties should become routine. Accurate phase diagrams and optical and magnetic properties of nanostructures should be possible for systems with more than thousands of atoms.

3. *What future scientific advances in computational materials research require cyberinfrastructure? Feel free to discuss research areas within the broad umbrella of materials research (includes condensed matter physics, materials science, and solid state chemistry) that may not be represented at the workshop. A) on a 5 year time scale; B) on a 10 year time scale.*

Designing nanoscale structures with desirable functional properties to be used as components in nanoscale electronics, nanoscale optoelectronics etc (5 -10 yrs).

Integrating the components into the device requires a fundamental understanding of contacting nanoscale structures (5 yrs).

To realize the potential of using nanostructure in device applications, large-scale fabrication of nanostructures with desired properties is required. One way of achieving this is through the process of self-assembly. The environment in which the self-assembly process takes place is important. For example, the self-assembly of nanostructures may be mediated by bio-colloidal materials. (10 yrs).

Fundamental issues on the mechanism of growth of nanostructures are not clearly understood. This requires long-time and large-scale quantum-mechanics based simulations (5-10 yrs).

Algorithms that exploit distributive computing to circumvent the limitation on the accessible simulation time in molecular dynamics. Such algorithm would allow long-time simulations for systems whose dynamics is dominated by infrequent events.

Marriage of bio-molecules (proteins, enzymes, DNA) colloids, non-bio materials (nanotubes, polymers, etc.) has great potential. Many bio-data bases exist, but little is done at the bio-nonbio materials interface (5 years)

4. *What elements of cyberinfrastructure are required for scientific advances in 3? A) on a 5 year time scale;*

Computer hardware (mainly FLOPS and memory speed/size) will have to increase with at least current Moore's law rates. Computational, storage and data transfer capacity need to be scaled up. Efficient parallel computing algorithms on machines with thousands or tens of thousands of processors need to become available. Enhanced affordable visualization needs to be present. The management of these resources needs to be improved. A computational material science grid needs to be developed.

Algorithm and theory advances are critical; these are part of cyber infrastructure. Algorithmic advances at least matching Moore's law will also have to be made. Monies for support of the people, not just the hardware are needed. Collaborative research teams with multi-disciplinary components are needed. Platforms are needed to inform the research community of the progress in the hardware and software. Data mining of computational results to find unappreciated regularities will be important.

Algorithms that exploit distributive computing to circumvent the limitation on the accessible simulation time in molecular dynamics. Such algorithm would allow long-time simulations for systems whose dynamics is dominated by infrequent events.

B) on a 10 year time scale.

There needs to be available efficient parallel computing algorithms on machines with tens to hundreds of thousands of processors. Computer hardware (mainly FLOPS and memory speed/size) will have to increase with at least current Moore's law rates.

Algorithmic advances at least matching Moore's law will also have to be made. Collaboration with computer scientists is crucial. There needs to be new mathematical advances in systematic up-scaling and coarse-graining methodologies. In computational materials design, improved exchange-correlation functionals are necessary for "interesting" modern materials, which are often strongly correlated

Computational materials design really isn't limited by available computing resources these days. Advances in theoretical methods will probably help out more than faster/more computers. Instead knowledgeable people thinking very hard are needed. Maybe this can be turned around to make a case for better training of students/postdocs.

There needs to be support for developed software and databases. The use of large data sets and data structures for similar materials will lead to rapid new synthesis techniques for materials with novel properties. File-sharing formats and standardized I/O are needed for multiscale research.

We need rigorous modeling of bio-materials; Kinetics and thermodynamics of multi-component alloys are needed. Advances depend on the modeling of real-life and biological systems, such as small-world models for networks, and evolutions.

5. *In your opinion, what emerges as the highest priority in your responses to 2 and 3?*

There is a diversity of computing needs beyond clusters, including high performance computational infrastructure. This needs to be easily available to needy researchers.

The highest priority is multiscale materials-by-design and multiscale modeling and modeling nano-bio-systems. The highest priority should be to achieve first-principles prediction and design of new functional materials (particularly of highly correlated systems, nano-molecular electronics and materials) and multiscale modeling of structure-microstructure-property relationships and the construction of various knowledge databases for complex systems.

The highest priority should be the development of high capacity data sharing, development of bio-materials databases, and data mining techniques. This will lead to much larger scale research in DMR.

The highest priority is continued funding for both algorithmic and software development and for advanced massively parallel computers. Software and algorithm development should be among the highest priorities.

Priority should be given to education of the materials research community about what is out there and what they can do with them. More resources need to be dedicated to producing highly educated people.

One needs a central research site to allow others to easily access the latest findings and algorithms.

Continued support for long-term group interactions, particularly interdisciplinary and ones that can lead to interplay between experiment and theory and interfacing among biology, colloid science and materials science.

6. *Please include any additional comments about Cyberscience and Cyberinfrastructure that you would like to make.*

- Cyberinfrastructure within materials research must be driven by the science.
- Cyberinfrastructure, and cyberscience within DMR, should not be defined too narrowly.
- DMR should have a healthy balance between hardware and people to advance cyberscience.
- DMR needs to make sure the program provides sufficient monies for graduate student and post-doctoral training, in addition to cyberinfrastructure.
- Interdisciplinary and cross disciplinary research must be encouraged to advance the science.
- The biggest contribution for, rather than ‘use of’, the cyberinfrastructure by physicists can be made through an analysis of its structure and dynamics (such as cyberinfrastructure stability, scalability, vulnerability, and optimization).
- It is important to study fundamental processes facilitated by ‘cyberinfrastructure’ using traditional ideas from, e.g. complex systems and statistical mechanics.

- Bridging the diverse time and length scales between the microscopic and macroscopic worlds is a crosscutting challenge in DMR.
- The interface between biology, colloid science, and materials science emerges as one priority area.
- We need real theorists, as well as computational physicists, who can see through the mass of numbers and algorithms and calculations to provide a better understanding of the nature of materials and processes.
- MCC is wonderful, keep up the good work. The variety and quality of the MCC posters were remarkable.
- Researchers need to rethink our mode of operation to advance cyberscience and cyberinfrastructure. For example, perhaps seriously consider commodity computing.
- One of the main stumbling blocks within materials research is the unmet need for better software engineering, and help for researchers to take their ideas from concepts and models to effective and efficient computational codes.

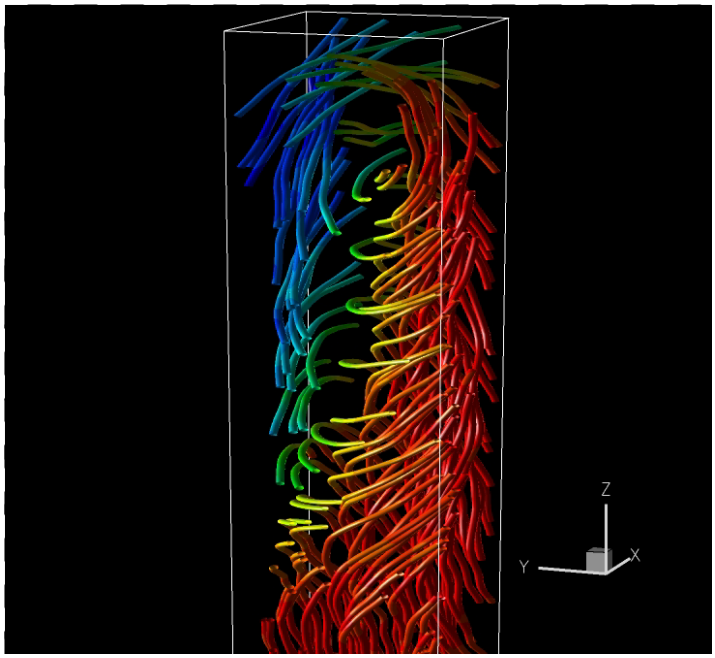

Figure 19. DMR-0120310. Stream lines showing a snapshot of the vorticity of the magnetization near one end of a nanoscale magnetic pillar. Nanoscale magnets are used in cyberinfrastructure for magnetic recording and for magnetic random access memory.