C. Project Description:

1. Motivation:

Three interrelated factors motivate this Materials Digital Library (MatDL) Pathway proposal: 1) the individual and complementary contributions materials science provides STEM education, 2) the onset of a new and rapidly evolving era of materials research, and 3) the rise of government funded, team-based materials programs across the academic MS community. By integrating materials science into the current portfolio of NSDL Pathway projects, MatDL Pathway proposes to build an information infrastructure to support education, research, and interactions between the two as well as to disseminate resources generated by government funded, team-based materials initiatives for the materials science community and its cognate fields of basic science, engineering, and mathematics (See Boeing letter of support).

The purpose of materials science (MS) is to improve the function, effectiveness, efficiency, and economy of products benefiting humanity by enabling component and system production (National Research Council (NRC), 1999). MS has a strong impact on all aspects of life including an estimated $400 billion yearly contribution of materials to the United States economy. The discipline originated most directly from metallurgy, ceramics and polymer science with important associations to other disciplines such as physics, chemistry, chemical engineering, geology, electronics, optics, and biology. The discipline blends pure and applied research by simultaneously pursuing both theoretical and practical objectives (Hessenbruch, 2002). Rather than taking a materials specific approach, MS can be conceptualized using five interrelationships (See Figure 1) basic for all kinds of matter (NRC, 1999): structure/composition, properties, performance, synthesis/processing, end-user needs and constraints.

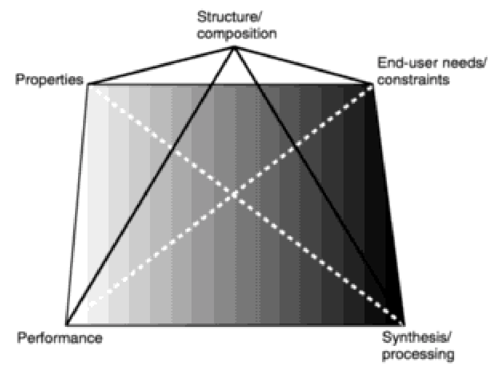

Figure 1. Connections among common elements in entire MS discipline including the end user. Source: NRC, 1999, p. 10.

Given its broad span, MS provides individual and complementary benefits to STEM education. As an individual discipline, MS emphasizes the study of the structure of materials (including metals, ceramics, semiconductors, polymers, and biomaterials) and of processing-structure-property relations that connect how a material is made to its end-use properties through the material's structure. An important undergraduate science program, MS encompasses a sizable student and faculty population as evidenced by the sixty ABET-accredited MS undergraduate programs offered at private and public institutions throughout the United States (Accreditation Board for Engineering and Technology (ABET), 2005). In addition, an increasing number of materials concentrations are being developed as part of undergraduate chemistry, physics and biology programs reflecting the field's impact on developments in bio- and nanotechnology. In support of biology, chemistry, physics, and the engineering sciences programs, new pedagogical approaches in MS teach the processing-structure-property relationships of real materials from the end-user's needs and constraints, incorporating economic, health, environmental, and manufacturing issues. With concentrations in MS, future biologists, chemists, physicists and engineers gain an understanding about how useful properties of a material can be modified by learning about the relationships between structure and properties as well as about the various chemical, thermal, mechanical, or other treatments to change and control structures.

The growing role of MS in STEM education reflects the world's entrance into a new and rapidly evolving era of materials research. New frontiers in MS include the fabrication of materials and composites to imitate human skin, muscles, bones, and neurons; the development of materials for new sources of power; and the design of materials at the micro-and nano-levels. (Rath, 2005). Nanoscience, a subfield of MS, has recently emerged as a fulcrum of national and international science policy. Researchers are pioneering the assembly of building blocks with unique structures and functions at the nanometer level that mimic biological self-organization processes as seen in proteins (Glotzer, 2004). These building blocks are "the 'atoms' and 'molecules' of tomorrow's materials, self-assembling into unique structures made possible solely by their design" (Glotzer, Solomon, & Kotov, 2004). Creating the next generation of molecular electronic, photonic, drug delivery, and sensing materials and instruments requires synthetic nanostructures that self-assemble with biomimetic precision. Developing a mechanism for precisely controlling assembly has been a major obstacle in fabricating these new materials and instruments. Recent simulation work has tested a promising strategy that uses attractive interaction sites or "patches" at specific surface locations of nanoparticles to cause the particles to self-assemble into predetermined ordered structures (See Figure 2) such as sheets, rings, square pyramids, and wires (Zhang & Glotzer, 2004; "Patchy Particles", 2004; "Patching together nanomaterials", 2004). Significant advances such as these underscore how the fundamental understanding of materials provides the basis for discovery of new materials.

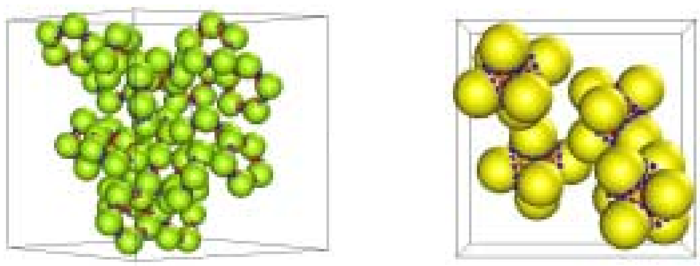

Figure 2. Examples of self-assembled nanostructures from functionalized nanoparticles, predicted by computational materials science techniques (Images provided by Zhenli Zhang (2005). Available: http://repository.matdl.org/handle/1862/1626 & http://repository.matdl.org/handle/1862/1623)

Given the broad impact of MS in areas such as medicine, electronics, and information technology, government agencies have increasingly supported the establishment of collaborative group efforts involving MS, such as NSF's *Materials Research Science and Engineering Centers* (MRSECs) (www.mrsec.org) and DOD's *Multidisciplinary Research Program of the University Research Initiative* (MURI) (http://www.onr.navy.mil/sci_tech/industrial/363/muri.asp). These multi-campus-based research centers address large and complex problems facing society by combining interdisciplinary, collaborative research with effective teaching and education of the wider community. The collaborative nature of these teams actively fosters data sharing and sponsoring agencies strongly encourage broad dissemination of centers' research and education. Currently, resource exchange and dissemination is primarily accomplished through individual team and program websites. Yet it is difficult to find organized resources from these group initiatives without going to each individual site. It is also time-consuming for centers to post recent research. In order to take full advantage of the resources available from these combined efforts, the centers need a common service that can be integrated into their existing workflow to archive and disseminate their information in an organized way as well as to promote discovery. Because of the impact of MS across STEM education, its role in development of new technology materials, as well as its contributions in government funded, team-based initiatives, the MatDL Pathway project within the NSDL can serve as a hub where different directions in MS can come together.

The National Academy of Science's landmark 1989 report, *Materials Science and Engineering for the 1990s: Maintaining Competitiveness in the Age of Materials* recommended strong, proactive, governmental support for MS given the pivotal role it plays across scientific communities and in the global economy. The report recommended uniting the broad constituencies involved in and affected by MS through enhanced communication, interaction, and coordination. Similar recommendations were made in the 2001 NAS report, *Materials in the New Millennium: Responding to Society's Needs.* Two of the five driving needs were: 1) the expansion of the basic knowledge base and 2) fulfillment of the education mission. These identified needs parallel the primary goals of the NSDL mission which include facilitating expansion of the STEM knowledge base, fulfillment of STEM education goals, and bringing together STEM communities. Meeting the challenges laid out by the NAS reports requires a collaborative and collective effort drawing together major parties in the MS community (See Section 1.2, Project Goals). The proposed MatDL Pathway project is well positioned to continue its efforts working with the MS community by providing a dedicated hub for the domain as well as offering the collective strategic advantages of the NSDL.

1.1. Targeted Audience

The long-term target community of MatDL is materials science undergraduate and graduate students, educators, and researchers. Given the multidisciplinary nature of materials science, the interests and needs of the materials community resonate across its cognate domains. In addition to the materials science community, a centralized repository of scientific visualization, codes, research results, homework assignments, and student work focusing on materials would be of benefit to biological sciences, chemistry, chemical engineering, mathematics, and physics.

1.2. Project Goals

The foundation for this MatDL Pathway proposal is our successful NSDL collection project (DUE-0333520). This project followed NSDL standards, implementing Dublin Core metadata and OAI harvesting, contributing collection as well as item level metadata to the NSDL Metadata Repository. All of the collection resources have Creative Commons or other digital rights attached. MatDL Pathway will continue these practices, working closely with NSDL Core Integration.

We seek to integrate MS as a domain and community into the portfolio of NSDL Pathway projects by building upon our collection project which identified and established relationships with a microcosm of the MS community in key areas: introductory undergraduate science courses, graduate education, as well as government and academic research groups. Partners included: Kent State University (KSU) the Materials Science and Engineering Laboratory (MSEL) at the National Institute of Standards and Technology (NIST), Massachusetts Institute of Technology (MIT), and the University of Michigan (U-M). MatDL Pathway will help to multiply the impact of NSF-supported materials efforts by expanding its existing collaborations to include three levels of the national and international MS community: *Nanoscale Interdisciplinary Research Teams* (NIRTs), *Materials Research Science and Engineering Centers* (MRSECs), and *International Materials Institutes* (IMIs). MatDL Pathway will integrate into the workflow of newly funded and established groups.

MatDL Pathway will design an information infrastructure to support education and research, as well as interactions between the two, such as adaptation of research data and code for educational purposes, with key representatives of the MS community as early adopters through their participation as co-investigators and collaborators. Social diffusion research indicates that unless a small number of respected community leaders first demonstrate the value of a new idea or behavior by acting as early adopters, the change is unlikely to spread throughout the community (Gladwell, 2000). In *Pasteur's Quadrant* (1997), Stokes noted that the separation of basic and applied research produces a strain on the "actual experience of science" while investment in Pasteur's quadrant of understanding-/use-inspired research can generate significant success for science and society. Others have correlated Stokes's argument to the separation of STEM research and education (Applegate, 2002; McHenry, 1998), and Borgman (2004) has extended this view by suggesting that "digital libraries have the potential to align the activities of scientists and students by providing context for the scientific process and by representing data in ways that are useful for multiple purposes".

Stewardship responsibilities for NSDL Pathway projects include supporting discovery, access, interoperability, reusability, and preservation. To facilitate the expansion of the basic MS knowledge base and fulfillment of the MS education mission, we propose to provide stewardship for content and services needed across the MS community and to provide a high quality educational experience for our targeted audience by offering:

1. Tools to describe, manage, exchange, archive, and disseminate data among national and international government-funded materials collaborations (teams and centers).
2. Workspace for open access development of modeling and simulation tools.
3. Services and content for virtual labs in large undergraduate introductory science courses.
4. Workspace for collaborative development of core undergraduate MS teaching materials as well as ontological tools for enhanced resource discovery.

2. Project Design:

To meet the four project goals, MatDL Pathway will provide the MS community with an open-source information infrastructure centered around Fedora (See Section 3) to support education, research, and interactions between the two. MatDL Pathway will collaborate with two key efforts in the MS community: 1) major MS initiatives including NSF-funded research programs such as NIRTs, MRSECs, and IMIs, as well as NIST/MSEL; and 2) innovative approaches to MS undergraduate education including virtual lab experiences for large introductory science courses and open archive environment for collaborative development of core MS teaching resources. MatDL will promote interactions between MS research and education in a variety of ways. For example, it will assist several NSF-funded materials research projects by disseminating Research Experiences for Undergraduates (REU) resources more widely through the NSDL. In addition it will help leverage investment in scientific data for educational purposes by facilitating the creation of learning objects from research data and code.

2.1. Major Materials Science Initiatives

Building collaborations with major MS initiatives such as NIRTs, MRSECs, IMIs, and NIST/MSEL lays the foundation to prepare research data and code for eventual submission in digital libraries, providing exciting opportunities to integrate recent research into teaching materials as they are being developed.

2.1.1. NIRTs, MRSECs, and IMIs

Nanoscience Interdisciplinary Research Teams (NIRT). NSF's NIRT program brings together small to medium-sized teams of materials researchers to carry out cutting-edge research on nanoscale science and engineering. Typical NIRTs are comprised of 3-6 principal investigators, half a dozen graduate students and postdocs, and several undergraduate students. Researchers in a single NIRT frequently come from multiple departments, different universities, and different locations. This multidisciplinarity and geographical distance pose unique challenges to the research team in sharing research tools and data as well as disseminating results. MatDL Pathway will work with a recently established NIRT with S. Glotzer (U-M) serving as co-PI on both projects. In addition to the Glotzer group, the NIRT involves research groups from three departments at North Carolina State University: MS (D. Brenner), Physics (J. Bernholc), Chemical Engineering (K. Gubbins, project PI. See NCSU letter of support) as well as Physical Chemistry (G.H. Findenegg) and Theoretical Chemistry (M. Schoen and S. Klapp) at the Technical University of Berlin in Germany. The goal of this NIRT is to simulate the behavior of surfactants on nanostructured surfaces and will require the sharing of datasets and nanostructures (See Figure 3) generated by the various groups using their own codes and data formats. An NSF SEIII proposal has been submitted for MatDL to provide the tools needed to support collaboration within distributed research groups such as the NIRT and with external collaborators such as the International Materials Institute Combinatorial Sciences and Materials Informatics Collaboratory (See following section on IMIs). In this Pathway proposal the emphasis is to

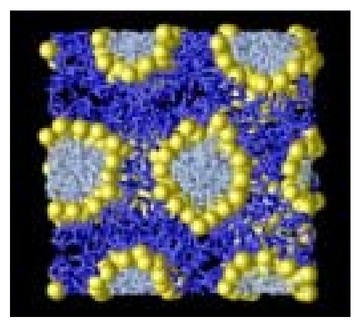

Figure 3. Example of self-assembled nanostructure predicted by computer simulation, representing a typical dataset that must be shared among NIRT collaborators. (Image provided by Sharon Glotzer)

make the NIRT's data publicly available in a centralized repository. MatDL will integrate Resource Description Framework Site Summary (RSS) into Fedora (See Section 3, Technical Design) to provide an alerting service based on individual selection criteria that facilitates data sharing among research group members. MatDL Pathway will also provide metadata expertise and the tools needed to submit the NIRT's data into MatDL, without duplicating earlier efforts. The NIRT will provide MatDL with data and nanomaterials information for access by materials educators, students, and other researchers. Furthermore, the NIRT will make additional information on nanostructured materials behavior available to the broad materials community by providing supplementary images and other simulation results beyond those published by the NIRT in standard journals. These resources will be used in graduate courses taught by Glotzer and Gubbins, and incorporated into and tested as a virtual lab experience with MIT's 3.091 course for use with 500 students (See section 2.2.1).

By working with the NIRT, we will be able to address within a manageable group some of the issues that face distributed research collaborations, such as strategies for data sharing. Because this NIRT is new, and members have not previously collaborated with each other formally, MatDL has the opportunity to work with them to establish effective data tagging and archiving strategies that will be built into their codes from the beginning. The NIRT will also serve as a testbed for larger MS collaborations described below.

Materials Research Science and Engineering Centers (MRSECs). The flagship centers for collaborative materials research funded by the NSF are MRSECs. There are currently 29 MRSECs at universities around the country, with a competition for new MRSECs currently underway. MRSECs typically involve on the order of two dozen faculty and their students from a single institution, as well as visitors and collaborators from other institutions. Several MRSECs are joint centers between multiple universities. A range of faculty expertise and backgrounds is typical of a MRSEC, with participation by as many as ten departments in addition to materials science and engineering. MRSECs serve as a focal point for materials education activities and are involved with a range of outreach and public education activities. Thus each MRSEC community is unique and diverse, representing a microcosm of the broader materials community.

The collaborative and diverse nature of MRSECs creates challenging materials data exchange needs on several levels. First, computational and experimental data must be shared among groups of faculty and their students working within the MRSEC on collaborative projects. Depending on how far along the research is, the researchers may wish to share this data with other MRSEC participants, or to make the data available to materials courses. After publication of their work, the researchers may wish to make their data available to the larger materials community or to outreach programs. MatDL Pathways will provide tools to describe and archive MRSEC resources for improved discovery in two ways. First, certain limited collections of materials data already generated will be described and archived on MatDL. Specifically, we will work with Cornell's well-established and successful MRSEC, Cornell Center on Materials Research (CCMR) (See Section 2.3.1). As a starting point of our work, we will broadly disseminate an important but manageable collection of existing REU papers and presentations from CCMR. Second, we will work with a new center being established by Co-PI Glotzer at U-M (potentially as a MRSEC, pending the outcome of the current competition) to build data tagging and archiving tools into their research model from the beginning. Types of data structures that will need to be archived include transmission electron, scanning electron, scanning tunneling, atomic force, and confocal laser scanning micrographs; x-ray and neutron scattering data; molecular simulation trajectories, and simulated microstructures.

International Materials Institutes (IMI). The NSF IMI program, currently comprised of six institutes, enhances international collaboration between U.S. researchers and educators and their counterparts worldwide. The Combinatorial Sciences and Materials Informatics Collaboratory (CoSMIC) is an established IMI directed by MatDL Pathway co-PI Rajan, whose mission is the demonstration and promotion of new methods of combinatorial experimentation, informatics, modeling and databases to dramatically enhance materials discovery and design using statistical techniques to accelerate discovery.

CoSMIC generates as well as collects both data and computer based data analysis and modeling programs, which are not copyrighted and which support both research as well as teaching. As a partner in the MatDL Pathway project, CoSMIC will submit these resources in an ongoing manner to MatDL, to provide broad dissemination of the IMI's research. These resources will also be used within the collaboration. For example, CoSMIC's materials informatics and data mining tools will be used to assist with analysis of the NIRT's simulation data of the behavior of surfactants on nanostructured surfaces. An NSF SEIII proposal has been submitted for MatDL to provide the tools needed to support collaboration within distributed research groups such as the NIRT and with external collaborators such as the CoSMIC IMI (See preceding section on NIRT).

In addition, CoSMIC will make available in MatDL its interactive teaching modules that can be used as a general on-line educational medium including:

Periodic Table teaching tool and materials science data: By applying statistical techniques to the entire periodic table CoSMIC has developed an interactive teaching tool for use with students to demonstrate that a wide range of information is available for all of these elements. This information includes their chemistry, engineering properties, and knowledge of how their atoms are arranged. CoSMIC's Periodic Table Tool (See Figure 4) will be incorporated into and tested as a virtual lab experience with MIT's 3.091 course for use with 500 students (See section 2.2.1).

Data based inquiry in materials science education: CoSMIC and the University of Tokyo have developed a joint teaching effort with a new course called *Molecular Design of Materials* at Rensselaer and a concurrent course on *Data Science* at the University of Tokyo, producing teaching materials, computer programs and other resources for teaching and education. CoSMIC with the University of Tokyo will incorporate the results of these efforts into the proposed MatDL Pathway project to develop an educational awareness of the mathematical principles on which these techniques are based through topics such as Principal Component Analysis, Partial Least Squares, Kernel Spectral Methods and Support Vector Machines.

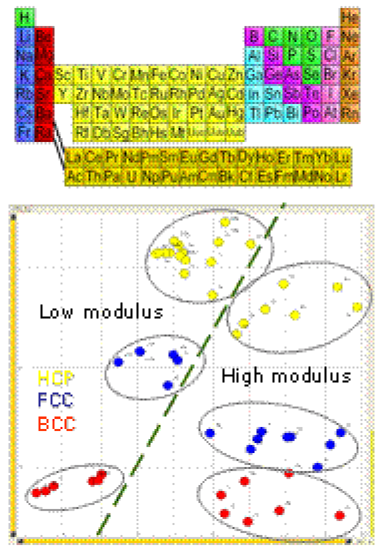

Figure 4. Image showing how the modulus characteristics of elements are clustered according to crystal structure based on data correlations derived from the periodic table. (Image provided by K. Rajan)

2.1.2. NIST MSEL CTCMS: Modeling & Simulation Code Developers

Development of tools and methods for the delivery of materials science digital information is the focus of research for the *Web Tools for Scientific Collaboration*, managed by the Center for Theoretical and Computational Materials Science (CTCMS) in the Materials Science and Engineering Laboratory (MSEL) of the National Institute of Standards and Technology (NIST). As part of its mission, CTCMS seeks new approaches to train students in the use of its tools, to promote development of its tools via testing, and to develop a pool of users ready to transfer the technology to industry and academia. Through collaboration between the *Web Tools* group and MatDL Pathway, CTCMS will pursue new methods to develop and disseminate its software tools, beginning with two software tools: FiPy and OOF. FiPy is an extensible, powerful, and freely available tool that is an object oriented, partial differential equation (PDE) solver, written in Python, based on a standard finite volume (FV) approach (Guyer, Wheeler, Warren, 2005). OOF is designed to help materials scientists calculate macroscopic properties from images of real or simulated microstructures (Langer, Reid, Haan, Garcia, & Roosen, 2004).

MatDL Pathway will integrate Subversion source control system into a Fedora-based infrastructure (See Section 3, Technical Design) creating a flexible workspace for NIST CTCMS and its external collaborators to use for "community" development of materials modeling and simulation codes, beginning with FiPY and OOF. The NSDL MatDL Pathway model for development and dissemination will offer clear advantages for government agencies such as NIST and other major MS initiatives over other currently available open source code development services, like SourceForge. As part of the NSF NSDL, MatDL Pathway will provide a branded, trusted, non-commercial, and neutral site supporting open source code development without the extensive security barriers that inhibit external collaborations required for servers residing within government institutions, such as NIST. By acting as a hub for research and education in the MS community, MatDL Pathway will promote interactions between research code developers and 1) other similar code projects; 2) researchers generating scientific data which could be used to test code; and 3) educators interested in incorporating the codes into teaching materials or in having students write code modules as part of their coursework (See Section 2.3.2). MatDL will also seek collaborations with other NSDL projects involved with software code in related areas, such as the Computational Science Reference Desk Pathway (CSERD).

2.2. Innovative Approaches to Materials Science Education

By collaborating with educators taking innovative approaches to MS undergraduate education such as developing virtual lab experiences for large introductory science courses and collaboratively developing shareable teaching resources for MS core courses, MatDL Pathway is embracing an opportunity to establish a digital library as an integral part of these activities by providing needed services and content and by facilitating interaction between the research and education elements of the MS community.

2.2.1. Introductory MS Undergraduate Courses & Virtual Laboratory

Laboratories represent a key component of undergraduate science coursework. In addition, engineering and computer science program accreditation necessitates demonstrated effectiveness of laboratory training (ABET, 2004). Yet the reality facing many science educators is the practical impossibility of providing meaningful lab experience in large introductory undergraduate science courses. Of the defined thirteen laboratory objectives (e.g., *experiment*, *data analysis*, *design*) at the ABET/Sloan Colloquy (Feisel & Peterson, 2002), at least three require physical presence in a lab: *instrumentation*, *psychomotor*, and *sensory awareness* (Rosa, 2003). Given forecasted growth in undergraduate enrollments and physical space limitations, online environments, such as digital libraries, may not only provide needed virtual laboratory support but also offer new opportunities for undergraduate science classes (Borgman, 2001). Under the MatDL collection project, a study was conducted during the January 2005 intercession at MIT to test the premise that a virtual laboratory (VL) could achieve the majority of learning objectives. The laboratory "experiments" were conducted in conjunction with data archived in the MatDL which also served as a repository for the reports and presentations authored by the students in the class. In all, eight students comprising two lab groups conducted three VLs. Self-assessment surveys taken before and after indicate that for many of the ABET expressed laboratory learning objectives the experience gave students a greatly improved understanding of concepts and mastery of skills covered in lecture (Bartolo, Lowe, Sadoway & Trapa, 2005). In a separate survey, students expressed positive opinions of the potential value of the MatDL collection project in supporting a virtual lab experience and in accomplishing additional educational objectives.

The current Pathway project proposes to examine scalability to determine if VLs can be offered to a class of 500 students, such as MIT's *Introduction to Solid State Chemistry (3.091)*. A key component of the proposed effort is the involvement of students as co-authors of the curriculum with the eight MIT students who took the intersession class invited to be part of the design and adaptation of the large-scale version. The workplan includes (1) enlarging the content of the VL through the development of a comprehensive set of experiments that resonate with the subject matter of the parent lecture subject (support for new content development will be sought through an NSF *Course, Curriculum, and Laboratory Improvement* (CCLI) proposal); (2) developing more elaborate assessment tools to measure the educational impact of the VL on the ABET learning objectives; (3) developing the infrastructure to allow the scale-up from a class of eight to a class of 500 to grow in stages: to 100 in year 1, to 200 in year 2, to 350 in year 3 and to 500 in year 4; (4) creating the capacity to modify the experiments so as to keep them new each time they are offered (student work products will be archived in MatDL and available to all to read so it is imperative that the course instructor be able to modify the lab exercise for future offerings.); (5) disseminating VL information and resources through MatDL and the NSDL Metadata Repository to instructors of large, freshman classes in chemistry, physics and biology to test for adaptability of the VL approach to other cognate domains.

MatDL Pathway will make available a variety of tested learning objects relevant to science educators interested in providing their students with a virtual lab experience. Example learning objects include: the Periodic Table tool and other materials from the IMI-CoSMIC (See Section 2.1.1, IMIs); reusable nanotechnology learning objects from the Pennsylvania State University (See PSU letter of support); and educational resources for core MS courses (See Section 2.2.2). It will archive nanotechnology research data from the NC State/U-M NIRT and U-M, which will be used to develop rich, new learning objects for a Self-Assembly VL in MIT's *3.091* course. A Resource Description Framework Site Summary (RSS) will be integrated into Fedora (See Section 3) to provide an alerting service about recent submissions that meet individual selection criteria. Additionally, MatDL will archive student output which will offer students new opportunities to extend their classroom experience with scientific information to licensing and publishing their own work as well as opportunities to benefit from work published by classmates.

2.2.2. Materials Science and Engineering Undergraduate Core

Educational resources for undergraduate core courses in the materials curriculum will form an important part of MatDL Pathway. Currently, there are entire classes of activities that could facilitate STEM education that are not available in the MS field as a whole. Outside of textbook publishing, there has been very little sharing among MS educators of pedagogical resources from homework problems and case studies to short handouts, and very little discussion of best practices in teaching specific topics to MS students. Resources for teaching MS topics to students of other disciplines represent another area that is unmet. Collaborative development and sharing of resources would greatly reduce the difficult and time-consuming tasks of preparing problems and assignments, writing handouts to explain difficult phenomena, keeping up with errata in textbooks, and authoring software to aid in teaching.

The MatDL collection project started work in this area by providing a Concurrent Version System (CVS) workspace for collaborative development of educational resources related to transport phenomena, with an initial focus on materials processing and performance. The Transport Phenomena Archive currently consists of more than 75 resources by four contributors of 57 problems, 11 handouts, four documents on pedagogy, one long (29-page) reading on fluid flow for graduate students, and three pieces of course-related software (http://mirl.lci.kent.edu/horde/chora/co.php/matml/transport/index.html?r=1.26). Resources were made more generally accessible by the addition of Dublin Core (DC) and Learning Object metadata (LOM) and through inclusion in the MatDL repository (http://repository.matdl.org/handle/1862/1469). A small transport phenomena ontology was also created to facilitate access to these resources.

MatDL Pathway will provide a more flexible workspace to facilitate the expansion of this initial work. Subversion source control system will be integrated into a Fedora-based infrastructure to enable support for file renaming and moving among directories, a controlled-access area for solution content, as well as tracking documents and software through submission, review, posting, and later revisions as necessary (See Section 3, Technical Design). Content of the original Transport Phenomena Archive is expected to expand to at least 1,000 resources incrementally over the next four years. An international Editorial Board is being assembled to review contributions with rigorous pedagogical standards for adoption and to steward the Archive into the future with support for the Board and resource contributions being sought through a NSF CCLI proposal. In addition to the CCLI-supported work, content will also expand to other course areas in MS. Powell, Krane, and Glotzer will provide resources from their home institutions by steering resources generated by colleagues teaching in core courses of the undergraduate materials curriculum into MatDL. Topics in the core at MIT, Purdue, U-M, and other Materials departments range from thermodynamics and kinetics to mechanical, electrical and biological materials to laboratory subjects. As an example, Prof. Rod Trice at Purdue has developed modules for an introductory materials course under his NSF Career award (DMR-0134286), which would be brought into MatDL. Powell, Krane, Glotzer, Rajan and Warren will also utilize connections to colleagues and societies, such as TMS (The Minerals, Metals and Materials Society) and MRS (Materials Research Society) to bring in relevant resources from other materials educators. Research data and software code made available in MatDL will also provide educators with essential components for creating powerful, new learning objects. MatDL Pathway will expand the existing transport phenomena ontology to include broader coverage required by core course topics, facilitating access to relevant resources across the collection.

2.3 Interactions between Research and Education

Two main areas of interactions between research and education will be addressed:

2.3.1 Research Experience for Undergraduates (REUs) Major MS research initiatives typically include an educational outreach component. For example, many MRSECs sponsor Research Experiences for Undergraduates (REU) projects (National Science Foundation, 2005) which support active research participation by undergraduate students in any of the areas of research funded by the NSF. While REU resources are currently available through individual project websites, it is difficult to locate resources across sites without going to each site separately. As a starting point, MatDL Pathway will more broadly disseminate existing REU output from two of Cornell University's materials research centers: Center for Materials Research (45 years in materials research; 16 years as REU project; 10 years as MRSEC) & NanoScale Science and Technology Facility (25 years in operation) (support indicated through telephone conversations and letters of support: CCMR Director of Educational Programs, Nevjinder Singhota; CNF REU contact, Dr. Lynn Rathbun). Existing REU student papers and presentations will be catalogued and made more accessible through MatDL and the NSDL Metadata Repository. Another outgrowth of this work will be the development of a model to determine the volume, type, and ongoing processing requirements for these resources. Once a model has been developed, it can inform decisions about working with materials centers to make REU output or other kinds of educational outreach materials available through MatDL. It might also assist other NSDL projects in forming similar arrangements with other research initiatives.

2.3.2 Leveraging Investment in Scientific Data for Education

In addition, MatDL Pathway will support leveraging investment for scientific data in major MS initiatives, such as adaptation of research data and code for educational purposes. Like the REU programs, many NSF-supported materials initiatives have websites about their individual projects but no easy access to all MS initiatives. Research data from the NIRT and IMI will be described, archived and made available on MatDL Pathway as soon as the data has been published or patent(s) awarded. These resources will carry Creative Commons or user-provided digital rights licenses. Research data from a proposed MRSEC will also be archived under the same arrangements. In addition, codes developed by NIST CTCMS and its external collaborators will be available for distribution on MatDL Pathway. Alert services from the NIRT, IMI, NIST CTCMS, and proposed MRSEC will notify the core MS teaching materials and the VL groups about available data. For example, the FiPy code can be incorporated by educators into their course materials for teaching students ordering processes in materials, while upper level undergraduates may use OOF modules as part of their course work.

3. Technical Project Design

While the MatDL collection project used DSpace as its repository infrastructure, MatDL Pathway plans to migrate to Fedora because of its numerous advantages in flexibility and customization as well as opportunities for collaboration with other projects using Fedora (See letter of support from Cornell Ornithology Laboratory). Fedora allows for a variety of metadata formats, all of which are searchable. The ability to associate MatDL resources with a variety of metadata schemas will provide many paths for resource discovery given the multidisciplinary nature of MS. Objects are versioned, which better supports preservation. Fedora also supplies an Application Programming Interface (API), which we will utilize to build custom interfaces. In migrating to Fedora, we plan to implement a user interface that allows any registered user to submit new items through the webpage. This requires us to add pages for registration, login, and submission to Fedora, along with an authentication scheme to regulate the new features. Pages for browsing and searching will also be added. Fedora also has the advantage of generalized object-to-object relations, which we hope to exhibit in the interface. For example, with this kind of flexibility, educators would be able to easily associate research output with their learning objects. To handle attribution and licensing, we will offer Creative Commons licensing or allow authors to use their own statements. We plan to package and make our customizations available to others through an install script.

We intend to use Subversion source control system and Resource Description Framework Site Summary (RSS) to enable groups to develop resources at the periphery of the repository. When the resources are ready for submission, the infrastructure will allow them to be easily moved into public view without duplicating effort. As an alternative submission process, Fedora will be connected with RSS 1.0 and Subversion. Fedora will act as a subscriber to RSS feeds. The RSS feed provides the metadata along with a reference to the item. Since RSS was not designed for digital libraries to receive, initially all submissions from RSS will be queued for human review before being put in the repository. Subversion is a natural tool for developers. Along with appropriate interfaces, we will provide space in Subversion repositories for group work, and a tool to migrate those items into Fedora. Along with the migration tool, the general repository will be added to Fedora through a redirect datastream. Since Fedora uses a more rich set of metadata than Subversion, it will be stored in a separate but similarly named file in Subversion.

Subversion and RSS will be used in MatDL to support integration of research and education. For example, we are planning to use RSS as a customizable alerting service. Taking a graduated approach, research group members in the NIRT and MRSEC will use RSS feeds with internal members as a way to describe and share emerging research. As their work matures, they will send the same feed to external collaborators, e.g., other NIRTs and MRSECs. When they are ready to make the research publicly available, MatDL will be alerted, signaling the onset of the automatic submission process. The VL developers and MS core teaching materials developers will receive the selected feeds as the resources are made available in MatDL. In addition, since RSS is a standard used by major publishers, MatDL will play an intermediary role helping to put publishable work in a ready format benefiting prospective authors and scholarly publishers.

4. Personnel and Management Plan

The assembled team on this proposal consists of highly qualified researchers and educators with a proven record of successful collaborations with one another as well as with others in the MS community. **Laura M. Bartolo, PI,** is Associate Professor, Materials Informatics Laboratory at Kent State University; PI of the current NSDL MatDL collection project; Co-PI of the past NSDL GREEN collection project. She co-chairs the NSDL Educational Impact and Evaluation Standing Committee; co-chaired the NSF/NSDL Workshop on Scientific Markup Languages held June 2004 at NSF; and will co-chair the NSDL/CODATA (Committee on Data for Science and Technology of the International Council for Science Unions) Workshop on Scientific Data, International Standards, and Digital Libraries to be held June 2005 at the Joint Conference on Digital Libraries. Bartolo will have primary responsibility for the overall direction of the Pathway project and will be the primary NSF contact. **Sharon C. Glotzer, Co-PI,** is Associate Professor of Chemical Engineering, Materials Science and Engineering, Macromolecular Science and Engineering, and Physics at the University of Michigan, and co-founder and former director of the NIST CTCMS. She is co-PI of the current NSDL MatDL collection project; PI of the proposed MRSEC; and co-PI of the NIRT project with which we will collaborate. She is a leading expert on soft materials simulation and computational nanoscience. Glotzer will be responsible for coordinating the work with the NIRT and U-M center. **Adam C. Powell, Co-PI,** is Thomas B. King Assistant Professor of Materials Engineering at MIT; co-PI of the current MatDL collections project and past NSDL Green's project; and will be responsible for co-coordinating the work of core MS teaching materials development with SI Krane. **Krishna Rajan, Co-PI,** is Professor of Materials Science at Iowa State University and PI of the current NSF International Materials Institute, CoSMIC. Rajan will be responsible for coordinating the work with IMIs. **Donald R. Sadoway, Co-PI,** MIT John F. Elliott Professor of Materials Chemistry, has 25 years' experience in teaching and curriculum development in undergraduate materials science subjects. Presently he is the instructor in charge of *3.091*, the largest class at MIT, a version of general chemistry that is taken by approximately 500 students every fall. Sadoway will be responsible for coordinating the work of Virtual Lab experiences. **James A. Warren, SI,** is Director, NIST MSEL CTCMS, and is an SI on the current NSDL MatDL collections project. Warren will be responsible for coordinating the work of NIST and external collaborators' code development. **Vinod K. Tewary, SI,** is Research Scientist, NIST MSEL Materials Reliability Division at Boulder, CO; CTCMS researcher; an SI on the current NSDL MatDL collections project and SI on the past NSDL Green's project. Tewary will be responsible for coordinating efforts on Green's functions. **Matthew J. Krane, SI,** is Associate Professor of Materials Science at Purdue University and will be responsible for contributing to and co-coordinating the work of core MS teaching materials development with Co-PI Powell. **Diane Geraci, SI,** is Director of Science Libraries at the University of Michigan and will advise on archiving issues and interactions with university science libraries. Two project meetings will be held each year (at rotating locations): one in Fall for PIs, SIs, project manager, and system manager; and one in Spring for PIs, SIs, their students, the project manager, system manager, and external evaluator. Team members will also communicate via email and teleconferencing throughout the project.

5. Timeline and Tasks

Year 1 • Collect technical requirements & variables to design framework & interfaces for:
- o Fedora-based infrastructure alerting service (Sect. 3, RSS) for NIRT (Bartolo, Glotzer)
- o Fedora-based infrastructure collaborative workspace (Sect. 3, Subversion) for NIST open source code developers (Bartolo, Warren)
- o Fedora-based infrastructure collaborative workspace (Sect. 3, Subversion) & ontology for core MS courses (Bartolo, Powell, Krane)
- o Domain specific, standards compliant metadata elements into NIRT codes (Sect. 2.1.1, Bartolo, Glotzer)
- o Digital library content & alert services (RSS) for VL experiences using IMI and other learning objects (Sect. 2.2.1,Bartolo, Sadoway, Rajan)

Year 2 • Prototype, evaluate & revise:
- o Fedora-based infrastructure alerting service (Sect. 3, RSS) of NIRT (Glotzer, Bartolo)
- o Fedora-based infrastructure collaborative workspace (Sect. 3, Subversion) for NIST open source FiPY code developers (Warren, Bartolo)
- o Fedora-based infrastructure collaborative workspace (Sect. 3, Subversion) & ontology for 200 MS course teaching materials (Sect. 2.2.2, Powell, Krane, Bartolo,)
- o Domain specific, standards compliant metadata elements into NIRT codes (Sect. 2.1.1, Glotzer, Bartolo)
- o Digital library content & services for VL experiences from IMI and other learning objects for 200 students (See Sect. 2.2.1, Sadoway, Bartolo, Rajan)

• Design Fedora-based infrastructure (RSS) at MRSEC (Bartolo, Glotzer)

• Catalog REU student presentations & papers for Cornell's CNF (Sect. 2.3.1, Bartolo)

Year 3 • Prototype, evaluate & revise:
- o Fedora-based infrastructure alerting service (RSS) at U-M site (Glotzer, Bartolo)
- o Fedora-based infrastructure collaborative workspace (Subversion) for NIST open source OOF code developers (Warren, Bartolo)
- o Fedora-based infrastructure collaborative workspace (Subversion) & ontology for 600 MS core course teaching materials using NIRT research data (Sect. 2.2.2, Powell, Krane, Bartolo)
- o Domain specific, standards compliant metadata elements into MRSEC codes and data (Glotzer, Bartolo)

- Digital library content & services for VL experiences from IMI and other learning objects for 350 students (Sect. 2.2.1, Sadoway, Bartolo Rajan,)

- Deploy Fedora-based infrastructure alerting service (RSS) in NIRT (Bartolo, Glotzer)
- Catalog REU student presentations & papers for Cornell's CCMR (Sect. 2.3.1, Bartolo)

Year 4 • Deploy:

- Fedora-based infrastructure alerting service (RSS) at U-M (Glotzer, Bartolo)
- Collaborative workspace & ontology for 1000 MS core course teaching materials using research data (See Sect. 2.2.2, Powell, Krane, Bartolo)
- Digital library content & services for VL experiences from IMI and other learning objects (See Sect. 2.2.1, Sadoway, Bartolo, Rajan) for 500 students

6. Sustainability

MatDL Pathway will maintain accessibility as formats, hardware, software, and platforms evolve. A robust digital library of ongoing research data and code will grow through MatDL's existing and proposed collaborations with MS research initiatives (NIRT, proposed MRSEC at U-M, IMI-CoSMIC, and NIST CTCMS). The repository of undergraduate MS teaching materials and student work will expand by working with innovative approaches to MS education through the proposed involvement with virtual lab experiences, collaborative teaching materials development workspace, and contributions from other MS education efforts, such as the Cornell CCMR REU and other efforts at Cornell and PSU (See also PSU letter of support). Partnering with key MS early adopters will ensure MatDL Pathway will keep in step with technology needs to support MS education and research. During the four-year period, MatDL will explore establishing a non-profit organization within the NSDL framework. Under such a model, sustainability would be pursued in two ways: 1) contract incremental parts of MatDL costs to MS research initiatives, such as NIRTs, MRSECs, IMIs for archival and dissemination services, and 2) partner with other MS related projects for external funding, such as innovative efforts in MS education. The fourth year funding for this proposal has a drop in support for core MatDL services to reflect the transition to other forms of support. In the long term, we envision NSDL MatDL as a non-profit group contracting work with MS research and education centers and also partnering with these groups for external funding. Organizations, such as MatDL Pathway and the NSDL, which are able to broadly disseminate resources as well as provide other needed services (e.g., archiving, preservation, conformance to accepted information standards, and guidelines to promote reusability), would benefit these centers by promoting resource discovery and by making more resources more accessible to a wider audience more quickly. This model could be extended throughout the NSDL to provide comparable services to other, large government-sponsored initiatives with similar research and education missions, which extend across the STEM domains. Such collaborations would leverage the collective strengths of the NSDL enabling users to take full advantage of the resources available from team-based efforts.

7. Dissemination

MatDL Pathway will use presentations, publications, and collaborations as a means of disseminating information about the project and the NSDL. Capitalizing on the multidisciplinary nature of the team, the MatDL collaborators will give presentations about MatDL Pathway and the NSDL at their respective societies. In the MatDL collections project, presentations about MatDL and NSDL were given at research and education sessions held by societies for digital libraries, library and information science, materials, metals, and physics (AIChE, APS, ASM, ASIST, CODATA, DC, ISKO, JCDL, MRS, TMS, and a IMI centers meeting). Publications related to the project appeared in numerous proceedings (Bartolo, Glotzer, Khan, Powell, Sadoway, Anderson, et al., 2004; Bartolo, Glotzer, Khan, Powell, Sadoway, Tewary, et al., 2004; Bartolo, & Lowe, 2003a; Bartolo, & Lowe, 2003b; Bartolo, & Lowe, 2003c; Bartolo, Lowe, & Glotzer, 2004; Bartolo, Lowe, Powell, Sadoway, Vieyra, & Stemen, 2004; Bartolo, Lowe, Sadoway, Trapa, 2005) and in several journals (Bartolo, Lowe, Feng, & Patten, 2004; Bartolo, Lowe, Sadoway, Powell, & Glotzer, 2005). Co-PI Sadoway and PI Bartolo gave a presentation on virtual lab experiences for large introductory courses at the 2005 APS (American Physical Society) meeting. PI Bartolo and the past President of CODATA are co-organizing a workshop about scientific data, international standards, and digital libraries to be held this summer at JCDL. In 2004, Co PI Powell and SI Krane co-organized a symposium at the TMS (The Minerals, Metals and Materials Society) Annual Meeting entitled *Educational Issues in Transport Phenomena in Materials Processing* that focused on the need for resources in order to facilitate teaching. Powell is organizing a symposium for the 2007 TMS Annual Meeting entitled *Internet and Other Electronic Resources for Materials Education* which will inform materials educators about resources available, such as MatDL and the NSDL, as well as how best to use them to meet educational goals Each member of the team has strong working relations with others in their respective fields. Through its team members, MatDL Pathway will expand upon the network of collaborators.

8. Evaluation

A third-party evaluation including both formative and summative components will be completed for this project. At each stage of the project, all collaborators have agreed to participate and to encourage their associates and students to participate in online surveys evaluating the following areas:

- Interface to the Fedora open source digital repository service
- RSS integrated into Fedora-based infrastructure to support data management and exchange among nationally and internationally distributed research groups,
- Subversion integrated into Fedora-based infrastructure to provide workspace for open access development of modeling and simulation tools as well as workspace for collaborative development of core undergraduate MS teaching materials.
- Services and content for VLs in large undergraduate introductory science courses
- Tools to describe, analyze, and archive data
- MS ontology for educational resources
- Research data being used to develop learning objects
- Students using/extending NIST codes

Usage data will also be collected in conformance with recommendations of the joint webmetrics taskforce of the NSDL Educational Impact and Evaluation Standing Committee & the Technology Standing Committee. The evaluation effort will be directed by Karin Tice, a partner at Formative Evaluation Research Associates (FERA). FERA (http://www.feraonline.com/) is an innovative evaluation group based in Ann Arbor, Michigan that has worked with non-profit organizations including libraries and universities for over 30 years. Dr. Tice established a relationship with the MatDL collection project by serving as its outside evaluator, attending bi-annual all-day group project meetings as well as interacting with the investigators by phone and email as needed. To date, FERA has provided MatDL with formative data from a collaborator survey (See Supplementary Documents, FERA) and a user survey. Although data collection for the user survey is still underway, responses gathered so far (from three undergraduate students and three research group members) generally express very positive opinions about MatDL and its potential value in accomplishing educational objectives, such as supporting a virtual lab experience. These surveys have collected information to help strengthen the initiative as well as documenting the preliminary impacts on students, faculty and researchers. MatDL Pathway will maintain regular communication with the evaluator to ensure that the project remains on track with its targeted goals and objectives. In addition to phone and email communication, an annual face-to-face meeting between the evaluator and the PIs will be conducted to discuss ongoing data collection and formative results as well as to plan and implement assessments.

9. Broader Impacts:

Two main areas of broader impact will be addressed:

Leveraging other funded efforts. Formal and informal collaborations between MatDL Pathway and several projects currently funded by NSF as well as additional projects currently under review by NSF and other agencies will multiply the impact of each effort on education and research. Collaborations with established and newly funded projects include: NIRT on nanostructured materials at North Carolina State University, MRSEC Cornell Center on Materials Research, two Cornell Nano centers (Cornell Center for NanoSystems and Cornell Nanosystem Facilities), and the IMI CoSMIC. Those currently in development or under review include: PSU's Nanotechnology Undergraduate Education (NUE), Co-PIs Powell and Krane's forthcoming CCLI for developing core MS teaching materials, Co-PI Sadoway's forthcoming CCLI for developing VLs and Co-PI Glotzer's submitted MRSEC proposal.

Developing models. A particular strength of MatDL Pathway collaboration is the support of material scientists in facilitating access to established materials-focused groups and in working together with information scientists to make a variety of quality MS resources accessible. The participation of materials scientists in making research data available presents a particularly exciting and unusual opportunity to expand digital library content to include non-traditional resources and to impact MS education. MatDL's experience could be used to develop models:

- of how other NSDL Pathways can work with other NSF-supported initiatives to multiply impact in their domain community
- for designing a digital library that provides the context for research & education to work together
- for handling existing & ongoing outreach by quantifying how much exists, as well as time, staff, tools required to get the resources into an NSDL repository
- for handling ongoing research data output by quantifying how much to store, how & how much detail to describe, what formats, how long before dissemination, etc.
- for quantifying time, staff, tools to turn research output into learning objects.

10. Results from Prior NSF Support

DUE-0333520 "Materials Digital Library: MatDL" ($808,574) Award Period - 9/1/03 - 8/31/05, PI: Bartolo Co-PIs: Glotzer, Powell, Sadoway SI: Warren, Tewary. The current NSDL collection grant tested a model focusing on MS content, tools, and users with a small representative subset of the MS research and education community. The project's accomplishments include: 1) submitted NIST MSEL research content available (e.g., Phase diagram collection, MALDI recipes, Polymer and combinatorial publications); 2) prototyped submission template to describe nanostructures in consistent and comprehensive way to improve data management and exchange in research group and to prepare for eventual submission to MatDL; 3) used image gallery in graduate classes to support comparison and archiving of students' work; 4) established archive of research data of nanostructures images; 5) conducted virtual lab experience for focused period with small group as preliminary work for large introductory undergraduate science courses with no lab. Students' presentations and papers submitted to MatDL and two surveys conducted showing students' positive assessment of learning improvements and potential value of MatDL in virtual labs; 6) established Transport Phenomena Archive for teaching materials described with DC and LOM metadata; 7) developed MatML grapher, a web based application which uses Materials Markup Language to create on the fly graphs comparing properties across materials 8) MatDL collection project has resulted in 12 presentations at national and international society conferences; 9 archival published papers; 5 submitted presentations; 4 submitted papers; 9) the project is scheduled to expose its metadata records for OAI-harvesting by the NSDL Metadata Repository in early May 2005 after courses have been completed at the collaborating partners' universities. 10) The MatDL Supplement award resulted in a well received NSF NSDL Scientific Markup Languages Workshop with 40 participants held at NSF; 11) John Rumble (CODATA) & Laura Bartolo (MatDL) will co-chair JCDL workshop on scientific data, standards, and digital libraries.

DUE-0121545 "Green's Functions Research and Education Enhancement" ($608,000) Award Period - 8/31/01 - 12/31/03, Co-PI Bartolo, Powell, SI Tewary. The GREEN Digital Library is a NSDL project. Results include (1) the "Green's Functions Experts Meeting" (2) a collection of Green's functions resources archived at http://appling.kent.edu/NSDLGreen/, (3) tutorials on Green's functions and Boundary Element Method (4) use of OAI metadata server to expose metadata records (5) XML document type description of Green's functions equations called GreenML, (6) specialized XSL stylesheet programs for IEEE-LOM and GreenML documents viewable at the GREEN site, (7) specialized GreenML editor (8) prototype GREEN taxon, thesaurus, and glossary. MatDL built upon GREEN by expanding the content for the collection, by using the content in education, and by providing domain specific authoring tools. Seven presentations & papers were delivered about the GREEN project.

DMR89-20147-12 "*School Based Remote Experiments on the Web*," ($160,058) Award Period - 8/31/98 - 9/1/02, Co-PI Bartolo. This project involved the NSF Science and Technology Center for Advanced Liquid Crystal Materials (ALCOM) Education Program, its industrial partners Keithley Instruments, Inc., Beta Micron, Inc., the Liquid Crystal Institute, and the Libraries at Kent State University. The results of the project: enabled schools to conduct real science experiments at a distance and assisted each participating school in providing unique science education resources to other schools. The teams integrated their experiments into information resources: 1) Collinwood High School, "Light, Polarization and Color", 2) John F. Kennedy High School, "LCD's and Magnetic Fields", 3) Magnificat High School, "Wind Tunnel", 4) Theodore Roosevelt High School "Reptilian Thermoregulatory Behavior", and 5) Southeast High School, "Crickets Trapped in the Web". Three presentations and two papers resulted from the *School Based Remote Experiments* project.

CTS-0210551, "NER: Simulation Strategies for Biomolecular Assembly of Nanoscale Building Blocks," ($100,000) Award Period - 08/01/02-07/31/04, PI S.C. Glotzer. Developed minimal models and efficient simulation strategies for simulating self-assembly of nanoparticles via biomolecule linkers. Developed a minimal lattice model of DNA- and antibody/antigen-directed nanoparticle assembly and simulated aggregation. Investigated the efficiency of various molecular and particle-based computational methods to simulate these models. A poster presented on this work by Ph.D. students T. Chen and M. Horsh and undergraduate S. Shah won 3rd prize in the 2003 AIChE Fall Meeting Poster Contest of the MSE Division out of 100 entries. Results were presented in a series of public Sigma Xi Distinguished Lectures by Glotzer, in nearly a dozen invited talks in 2003-2004, and in several publications (Lamm, Chen, & Glotzer, 2003; Chen, Lamm, & Glotzer, 2004; Glotzer, 2004; Glotzer, et al., 2004).

DMR-0103399 "NIRT- Multiscale Simulation of the Synthesis, Assembly and Properties of Nanostructured Organic/Inorganic Hybrid Materials," ($1.95M) Award Period - 8/1/01-07/31/05, Co-PI S.C. Glotzer. Developed mesoscopic models of silica nanocubes functionalized with organic tethers, and simulated this model using molecular simulation methods. Predicted nanostructures formed via self-assembly of monotethered and tetratethered POSS silica cubes due to immiscibility of tethers and cubes. Results appeared in and on the cover of the August 2003 issue of Nano Letters and was featured in a NY Times article in December 2002. For Glotzer group, one invited article is in press (McCabe et al.), one full research article (Chan et al.) and two conference proceedings (Zhang, et al. and Glotzer, et al.) are in press, and two full research articles are in preparation. First place, Materials Research Society Fall Meeting Poster Session, December 4, 2003, Boston, MA. (Zhang, X. et al., 2003)

DMR-0315603 "IMR: Acquisition of a Beowulf Computer Cluster for Materials Research and Education," ($200,000) Award Period - 08/15/03 to 09/15/04. PI S.C. Glotzer, Co-PIs Kieffer, Falk, Larson. The co-PIs recently acquired a 320 dual-processor Apple G5 compute cluster for materials simulation. The cluster supports research in four faculty research groups.

DMR-0231291 Combinatorial Sciences and Materials Informatics Collaboratory (CoSMIC-IMI) Rajan ($3,550,000) Award Period - 2/01/03 - 1/31/08. The resources of this center will be leveraged into this program, including large scale computational resources. The database, computational infrastructure along with its international outreach program will be a major leveraging support for this project. The CoSMIC-IMI has set up a materials informatics web portal (http://cosmic.rpi.edu), a international program for supporting graduate students and visiting scientists to work in our center, published dozens of papers, hosted numerous international workshops and meetings, and graduated the first set of PhDs majoring in materials informatics.