ARTICLES

D-Lib Magazine
March 2005

Volume 11 Number 3

ISSN 1082-9873

NSDL MatDL

Exploring Digital Library Roles

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Abstract

A primary goal of the NSDL Materials Digital Library (MatDL) is to bring materials science research and education closer together. MatDL is exploring the various roles digital libraries can serve in the materials science community including: 1) supporting a virtual lab, 2) developing markup language applications, and 3) building tools for metadata capture. MatDL is being integrated into an MIT virtual laboratory experience. Early student self-assessment survey results expressed positive opinions of the potential value of MatDL in supporting a virtual lab and in accomplishing additional educational objectives. A separate survey suggested that the effectiveness of a virtual lab may approach that of a physical lab on some laboratory learning objectives. MatDL is collaboratively developing a materials property grapher (KSU and MIT) and a submission tool (KSU and U-M). MatML is an extensible markup language for exchanging materials information developed by materials data experts in industry, government, standards organizations, and professional societies. The web-based MatML grapher allows students to compare selected materials properties across approximately 80 MatML-tagged materials. The MatML grapher adds value in this educational context by allowing students to utilize real property data to make optimal material selection decisions. The submission tool has been integrated into the regular workflow of U-M students and researchers generating nanostructure images. It prompts users for domain-specific information, automatically generating and attaching keywords and editable descriptions.

Introduction

Recent workshops and forums have held provocative discussions about the roles digital libraries can play as part of the emerging cyberinfrastructure/e-science [1, 2]. To advance discovery, learning, and innovation in the scientific enterprise, common themes throughout the discussions included:

- Knowledge specific communities,
- Collection and exchange of data, and
- Support for research and education.

In keeping with this discourse, the Materials Digital Library [Note 1], as part of the NSF National Science Digital Library program, investigates an information infrastructure for the materials science community that facilitates integration of research and education as well as advancement of the individual goals of each. MatDL is a collaborative effort involving materials scientists at the Materials Science and Engineering Laboratory at the National Institute of Standards and Technology (NIST), Massachusetts Institute of Technology (MIT), and the University of Michigan (U-M) with computer and information scientists at Kent State University (KSU) and the University of Colorado (CU) [Note 2].

Materials science (MS) represents an important intersection in the scientific community because of the central and complementary role it plays in STEM (Science, Technology, Engineering and Mathematics) research and education. Inherently multidisciplinary, materials science is making advancements toward the design and generation of novel materials with desired properties, such as the self-assembly of nanostructures [3]. Recognizing the pivotal position that materials science holds across scientific communities and in the global economy, the landmark 1989 report, *Materials Science and Engineering for the 1990s: Maintaining Competitiveness in the Age of Materials* [4], recommended uniting broad constituencies involved in and affected by materials science and engineering through enhanced communication, interaction, and coordination. Two of the five driving needs that the committee identified were: 1) the expansion of the core knowledge base and 2) fulfillment of the education mission. Meeting these challenges requires a collaborative and collective effort bringing together major parties in the materials science community.

A key mission of the National Science Digital Library Program (NSDL) is to bring together groups within the scientific community to enhance discovery, learning and innovation by facilitating greater integration of research and education. Borgman [5] has proposed that challenge of designing scientific digital libraries that simultaneously support research and education requires:

- Leveraging scientific data investment,
- Using inquiry learning to improve science instruction, and
- Offering services for data use and exchange.

As a project within the NSDL, MatDL addresses these priorities with the materials science industrial, research, and teaching community by examining the roles digital libraries can play in:

- Supporting virtual laboratories in large introductory undergraduate science courses without physical labs,
- Developing markup language applications to support research and education, and
- Building tools to meet materials scientists' requirements for data collection and exchange.

NSDL MatDL: Exploring Roles within the MS Community

Supporting virtual laboratory experiences

Laboratory experience has long been considered a critical component of all undergraduate science coursework. In addition, engineering program accreditation [6] requires that programs provide their graduates with training to demonstrate certain abilities, such as the capacity to design and conduct experiments. Traditionally, these abilities have been developed through physical laboratory training. However, there are many practical difficulties associated with providing meaningful hands-on lab experience, especially in large introductory undergraduate science courses.

Online environments, such as digital libraries, may offer both needed assistance and new opportunities by supporting virtual lab experiences for introductory undergraduate science classes [7]. Many of the current obstacles related to offering physical labs, such as dwindling budgets, limited physical space, and forecasted increases in undergraduate enrollments may be alleviated or minimized, if the same instructional objectives of a physical laboratory experience can be achieved through a virtual lab. The ABET/Sloan Colloquy [Note 3] suggested that creating an inquiry-based, collaborative learning experience may be more important than whether the experience is physical or virtual [8]. The colloquy identified thirteen engineering laboratory learning objectives (i.e., *instrumentation, models, experiment, data analysis, design, learn from failure, creativity, psychomotor, safety, communication, teamwork, ethics in the lab, sensory awareness*) that can be used to assess achievement for both physical and virtual laboratory experiences. It has been suggested that many of these objectives can be achieved outside of a physical lab, with some exceptions (such as, *instrumentation*, *psychomotor*, and *sensory awareness*), and that objectives fall into a hierarchy of importance [9]. *Ethics*, *data analysis*, *communication*, and *teamwork* were considered essential. *Models*, *experiment*, *instrumentation*, and *safety* were considered very important. *Sensory awareness*, *psychomotor*, *learn from failure*, and *design* were considered important.

MatDL investigators at MIT and KSU conducted student surveys to begin to address questions concerning the effectiveness of a virtual lab as well as the potential value of a digital library in supporting the experience [10]. A small group (8) of MIT students taking *Solid State Chemistry Virtual Laboratory* were asked to assess change in their understanding (1 = significantly worse, 3 = no change, 5 = strong improvement) of the 13 ABET laboratory objectives as a result of the virtual laboratory experience. The virtual lab was offered during a special four week Independent Activities Period (IAP) to students who had previously completed an introductory chemistry course. Survey results indicated students thought that the virtual lab was successful in improving their understanding of many of the 13 ABET laboratory objectives, with the most perceived improvement being associated with *experimental*, *team work*, *ethics in research*, and *communication* (Means 4.50, 4.50, 4.63, 4.75, respectively) . These early results support the opinion that some lab objectives may be successfully achieved through virtual lab experience [9]. Three objectives that were associated with the most perceived improvement (*team work*, *ethics in research*, and *communication*) have been identified as essential objectives of the laboratory experience.

A goal of MatDL is to archive scientific research data so that science faculty can provide their students with realistic data in order to accomplish laboratory objectives, including data analysis and report writing. In addition, MatDL offers students new opportunities to extend their classroom experience with scientific information to licensing and publishing their own work. A subset (3) of the MIT group of students also completed a survey that gathered opinions about MatDL's potential value (1 = very valuable, 3 = somewhat valuable, and 5 = not at all valuable) in accomplishing eight educational objectives [10]. In general, students expressed positive opinions with responses ranging from 1 to 3 (see Table 1).

Table 1. Student assessment of MatDL potential value in supporting 8 educational objectives

MathDL Educational Objectives	N	Mean	Std. Deviation
Support a virtual laboratory experience	3	1.33	.57735
Give students practical experience with publishing their own work	3	1.33	.57735
Give students practical experience with licensing their own work	3	1.33	.57735
Support work/interaction with students enrolled in similar courses at other institutions	3	1.33	.57735
Increase student awareness of research applications in materials science	3	1.33	.57735
Give students access to classmate's publications	3	1.66	.57735
Increase student interest in research	3	2.00	1.0000
Make courses more interesting by making available related research data	3	2.00	1.0000

They expressed a very positive estimation of MatDL's potential to support a virtual laboratory experience and a similarly positive view regarding its potential to give students practical experience with licensing and publishing their own work; to support interaction with students at other institutions; and to increase student awareness of applications in materials science (all *M* = 1.33). Students were also quite positive about MatDL's potential to give students access to classmate's publications; increase student interest in research; and make courses more interesting by making available related research data (Means 1.66, 2.0, 2.0, respectively). These preliminary results suggest that students view MatDL as potentially valuable in supporting a variety of educational objectives, including a virtual lab experience. Additional responses to this survey are currently being gathered from other groups.

Developing markup language applications

Digital libraries can play an important role within their domain communities in supporting the advancement of internationally accepted standards for reliable exchange of information, like scientific data. As an example, quick, easy access to materials property data is of critical importance in all segments of the materials community. There have been numerous initiatives involving private industry, government laboratories, universities, standards organizations, and professional societies to address this need. A case in point is the Materials Property Data Markup Language (MatML), an XML application originally developed at NIST. The markup language is expressly designed for the management and exchange of materials information [11] by facilitating automated use of data and resolving data interpretation and interoperability difficulties.

Because few examples using MatML were widely available, MatDL undertook a pilot [12] to provide a practical model in order to investigate use of a common data format by the materials community. The pilot supplies materials property data to a web-based application program that enables students to generate graphs comparing selected properties across various materials. The intent of the pilot was to explore benefits and obstacles relating to widespread adoption in academe, government, and industry by: 1) tagging (see Figure 1) materials property data with MatML, 2) parsing MatML files, and 3) developing a markup language web-based application for e-learning.


```
<Material>
<BulkDetails>
<Name>Titanium, TI</Name>
<PropertyData property="pr13">
<Data format="float">435.4</Data>
</PropertyData>
</BulkDetails>
</Material>
<Metadata>
<PropertyDetails id="pr13" type="thermal">
<Name>Heat of Fusion</Name>
<Units name="J/g" description="Joules per gram">
<Unit Description="Joules">
<Name>J</Name>
```

```
            </Unit>
        <Unit power="-1">
            </Unit>
         </Units>
    </PropertyDetails>
 </Metadata>
```

Figure 1. Partial example of MatML applied to titanium materials property data.

MatML was applied to a database of property data for 80 materials covering ceramics, metals, and polymers. The markup language is being used as the data input format with the web-based application that generates graphs showing selected properties for the different materials. The DOM [Note 4] extension in PHP [Note 5] is used to parse all the MatML files in the materials directory. The entire file is not parsed, but instead XPath [Note 6] is used to search for a set of properties related to the current graph. The points and material names for the graph are cached in a session variable until the axes change, which is then displayed as a scatter plot by using the image functions in PHP.

The pilot focuses on an exercise in a core requirement course for MIT materials science undergraduates, *Materials Processing*, MSE 3.185, which covers broad topic areas such as diffusion, heat conduction, fluid flow, and coupled transport. Traditionally, students have considered the course to be difficult given the breadth of the syllabus and complexity of the topics.

In the original exercise (see Figure 2), students were given the values of thermal conductivity, density, and heat capacity for a short list of materials. The learning objective of the assignment was for students to be able to select the best material for six different purposes based on the property data provided.

1. Thermal properties and optimal materials selection (27)

In many situations, product designs include parts whose only function is to conduct or resist the conduction of heat. Materials for these parts are thus chosen entirely on the basis of their thermal properties. Select the best material from the list provided for each of the following applications.

(a) Heat shield sandwiched between a hot body and a cold one which minimizes the steady flux between them. (4)

(b) Heat shield which protects something from short, intense bursts of heat (long timescale is needed). (4)

(c) Cheap (i.e. not diamond) temperature sensor, in which short timescale of heat conduction is necessary for rapid response. (4)

(d) Light heat reservoir which must hold as much heat as possible per degree C per unit weight. (4)

(e) Heat sink for a semiconductor device, which must minimize temperature difference for a given flux. (4)

(f) Heat sink for melt spinning, in which liquid metal is injected against a rotating heat sink where it is solidified as rapidly as possible, so the material must conduct heat away from the surface quickly. (Hint: evaluate the flux through $x = 0$ in an erfc-like unsteady conduction problem. Diamond is not an ecomonically viable option.) (7)

Candidate materials:

Material	k, $\frac{W}{m \cdot K}$	ρ, $\frac{g}{cm^3}$	c_p, $\frac{J}{kg \cdot K}$
aluminum	238	2.7	917
copper	397	8.96	386
gold	315.5	19.3	130
silver	425	10.5	234
diamond	2320	3.5	519
graphite	63	2.25	711
lime (CaO)	15.5	3.32	749
silica (SiO_2)	1.5	2.32	687
alumina (Al_2O_3)	39	3.96	804

Figure 2. Example of old exercise on materials selection based on thermal properties.

In the new web-based application exercise that eliminates time and effort constraints required to perform manual calculations, students are able to experiment with more materials and analyze the results presented as a graph. A survey with the students is planned to determine whether the graphical display (see Figure 3) made it easier for students to identify property differences between materials, to see patterns emerge, to make judicious substitutions between properties of comparable materials, and to be aware, as future engineers, of the potential value of web-based technologies, such as markup languages.

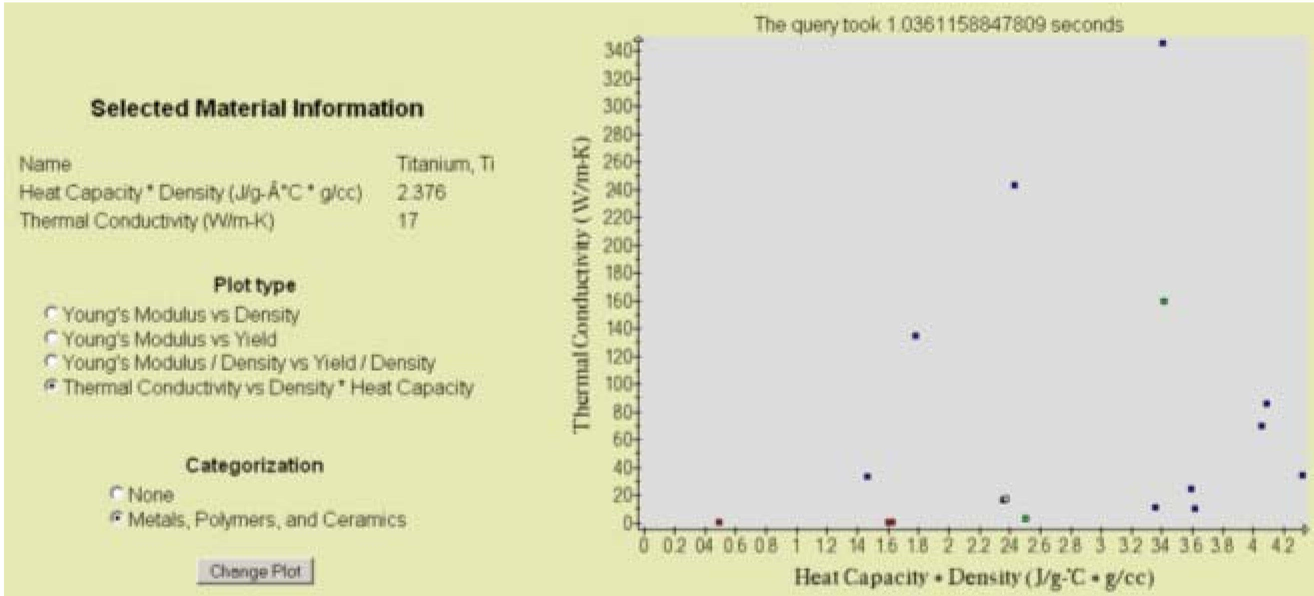


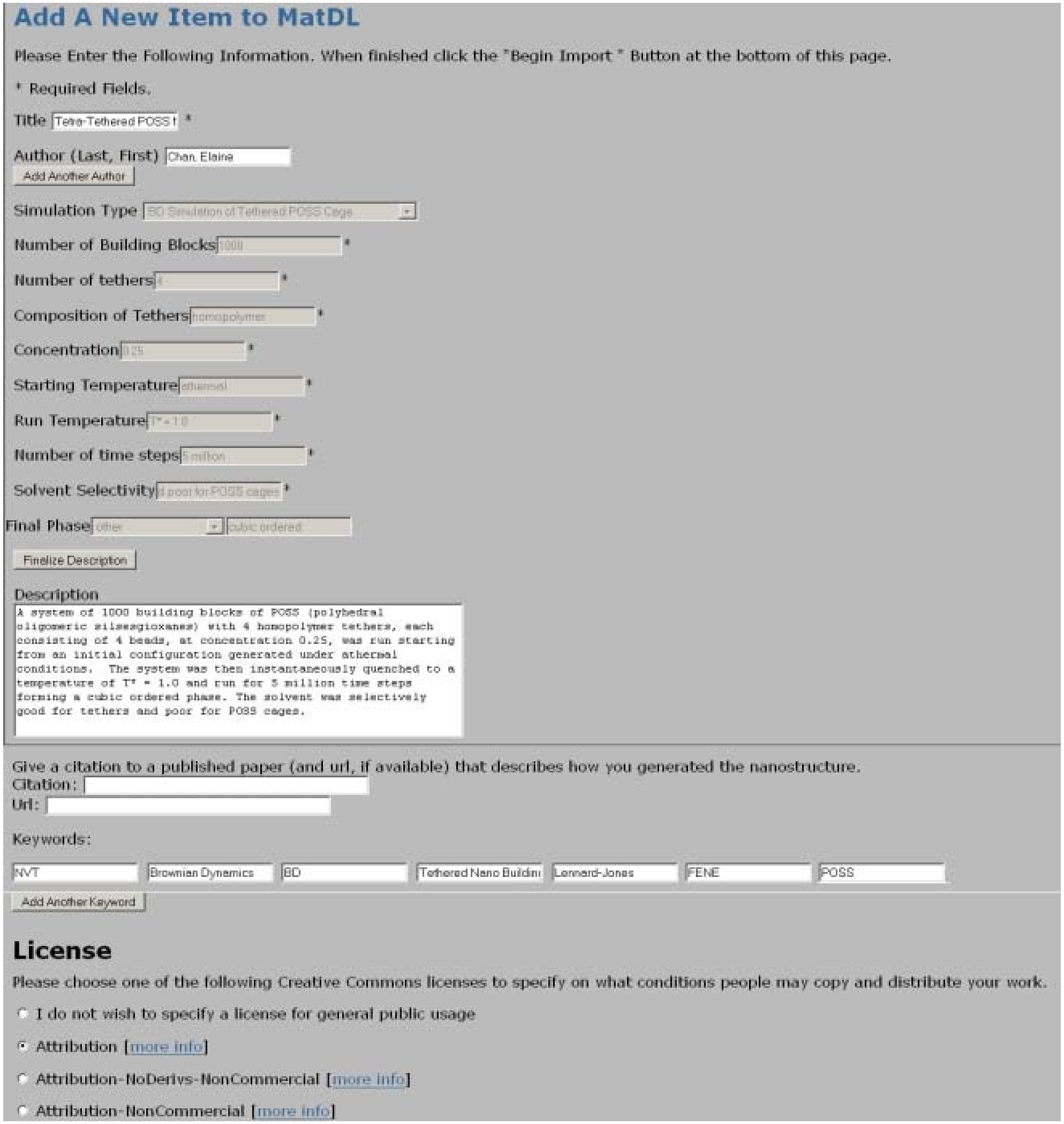
Figure 3. Sample graph of multiple materials with specific property values for Titanium.

The potential impact of the pilot can be beneficial to a broad range of constituencies in the materials community. Educators may adapt the pilot to develop new exercises and applications pertinent to materials processing. Researchers may employ the model for the reliable exchange of materials data with simulation software, such as NIST's Object-oriented Finite Element (OOF), that performs virtual experiments to measure and visualize internal stresses [13]. Industry may use the model for storing, communicating, and retrieving material data in a variety of industrial settings, such as for use with computer assisted design software to choose material for performance across temperature range or to optimize the composition for a particular function.

Building tools to meet requirements for data collection and exchange

By supporting reliable collection and exchange of data, digital libraries can fulfill a key role within their domain communities both for researchers generating data to advance research as well as for faculty using the data with their students to advance learning. MatDL is exploring this role through collaboration between information scientists at Kent State University and materials scientists at the University of Michigan whose research focuses on computational nanoscience and soft matter simulation. This work produces a rich array of nanostructure images. The goal of the collaboration is to capture metadata that reflects the kind of simulation details that materials scientists need to understand and replicate the simulation. The resulting metadata is intended to improve resource retrieval both within a single lab as well as a within a distributed network of collaborating labs. Attaching description to the data at the time of collection also produces additional advantages. Removing major barriers for submitting resources to outside repositories, such as digital libraries, greatly increases the likelihood that the user will make contributions to user-sustained repositories. Furthermore, once the resources reach outside repositories, they may be adapted for additional purposes, such as education.

To facilitate metadata capture, MatDL is developing a nanostructure submission template (see Figure 4) that is being piloted and tested as part of a research group's regular workflow.



Add A New Item to MatDL

Please Enter the Following Information. When finished click the "Begin Import " Button at the bottom of this page.

* Required Fields.

Title [Tetra-Tethered POSS f] *

Author (Last, First) [Chan, Elaine]

[Add Another Author]

Simulation Type [BD Simulation of Tethered POSS Cage]

Number of Building Blocks [1000] *

Number of tethers [4] *

Composition of Tethers [homopolymer] *

Concentration [0.25] *

Starting Temperature [athermal] *

Run Temperature [T* = 1.0] *

Number of time steps [5 million] *

Solvent Selectivity [d poor for POSS cages] *

Final Phase [other] [cubic ordered]

[Finalize Description]

Description

```
A system of 1000 building blocks of POSS (polyhedral
oligomeric silsesgioxanes) with 4 homopolymer tethers, each
consisting of 4 beads, at concentration 0.25, was run starting
from an initial configuration generated under athermal
conditions.  The system was then instantaneously quenched to a
temperature of T* = 1.0 and run for 5 million time steps
forming a cubic ordered phase. The solvent was selectively
good for tethers and poor for POSS cages.
```

Give a citation to a published paper (and url, if available) that describes how you generated the nanostructure.

Citation: [ ]

Url: [ ]

Keywords:

[NVT] [Brownian Dynamics] [BD] [Tethered Nano Buildin] [Lennard-Jones] [FENE] [POSS]

[Add Another Keyword]

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Figure 4. Submission template for nanostructures

The current version of the tool prompts users for all parameters associated with a static list of simulation types (e.g., *BD simulation of a tethered POSS cage, DPD simulation of a block copolymer*), capturing the values necessary to recreate the simulation. The parameters displayed are dependent on the simulation type selected. For example, the *Brownian Dynamics simulation of a tethered POSS cage* simulation includes prompts for: number of building blocks, number of tethers, composition of tethers, concentration, starting temperature, run temperature, number of time steps, final phase, and solvent selectivity. The *Dissipative Particle Dynamics simulation of a block copolymer* simulation shares some of the same parameters (e.g., number of building blocks, concentration, run temperature, number of time steps, and final phase), and also requires a prompt for Delta A. The simulation type selection also causes simulation method and model, as well as keywords to be automatically generated. An editable description paragraph incorporates all of the entered parameter values. When finished, users submit the domain specific metadata to the MatDL repository along with appropriate images, data files, and licensing (see Figure 5). Currently, users may submit a resource that is not represented on the list of simulation types, but at the cost of losing the convenience of detailed prompts as well as automatic keyword and description paragraph generation. Development of a flexible template is planned to better accommodate the parameter variability associated with a range of simulation types.

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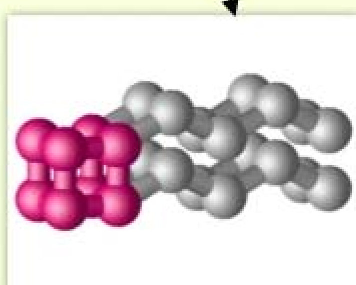
Lab for Computational Nanoscience and Soft Matter Simulation >

Please use this identifier to cite or link to this item: http://hdl.handle.net/1862/1630

Title:	Tetra-Tethered POSS Micelles 2
Authors:	Chan, Elaine
Keywords:	NVT Tethered Nano Building Block POSS Brownian Dynamics Lennard-Jones BD FENE
Issue Date:	31-Jan-2005
Description:	Simulation Software: Glotzer Group Code Simulation Method: Brownian Dynamics A system of 1000 building blocks of POSS (polyhedral oligomeric silsesgioxanes) with 4 homopolymer tethers, each consisting of 4 beads, at concentration 0.25, was run starting from an initial configuration generated under athermal conditions. The system was then instantaneously quenched to a temperature of T* = 1.0 and run for 5 million time steps forming a cubic ordered phase. The solvent was selectively good for tethers and poor for POSS cages. Simulation Model: United Atom Bead Spring with Lennard-Jones and FENE
URI:	http://hdl.handle.net/1862/1630
Appears in Collections:	Lab for Computational Nanoscience and Soft Matter Simulation

Files in This Item:

File	Description	Size	Format	
tetra-tether-poss-4bead-zoom-new.jpg	Single nanobuilding block	38Kb	JPEG	View/Open
4bead-Micelle-M10.tiff	Spherical micelle with 10 NBBs	1647Kb	TIFF	View/Open



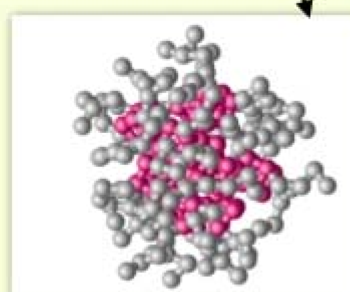


Figure 5. MathDL item record of submission

In addition to the research group, versions of the template have also been successfully used with a graduate class [14, 15] where students generated images of nanostructures through simulation codes to gain an understanding of how the structures were assembled. While the template assists authors in producing more complete and consistent metadata, a more seamless approach would be to capture the metadata directly from the simulation software, eliminating an extra step for authors and reducing the possibility of error. As a next step, MatDL plans to semi-automate metadata capture by writing metadata generation scripts that can work with simulation codes.

Discussion

Digital libraries can play numerous roles in the emerging cyberinfrastructure/e-science [1, 2]. MatDL has recently explored supporting virtual laboratories in large introductory undergraduate science courses without physical labs. Early student self-assessment survey results expressed positive opinions of the potential value of MatDL in supporting a virtual lab and in accomplishing additional educational objectives. A separate survey suggested that the effectiveness of a virtual lab may approach that of a physical lab on some of the 13 ABET laboratory objectives [8]. MatDL has also explored developing markup language applications by creating an educational application that utilizes MatML-tagged materials property data. The program generates graphs allowing students to easily compare selected materials properties across numerous materials. Finally, MatDL has investigated building tools to meet materials scientists' requirements for data collection and exchange by developing a nanostructure submission template to support the capture of detailed domain-specific metadata.

By collaborating with research groups, such as a nanoscience simulation group at the University of Michigan, to capture detailed metadata, MatDL can facilitate data use and exchange within individual labs as well as groups of collaborating labs. At the same time, MatDL can help leverage investment in scientific data by preparing the data for eventual submission to outside digital libraries and by supporting reuse of the data in an educational context. For example, there is considerable interest in using research data generated by the nanoscience simulation group to expand MIT students' inquiry-based, virtual lab experience. The web-based application using MatML provides an additional example demonstrating the types of services that can be developed in support of data use and exchange. The application provides proof of concept, demonstrating the benefits of a common data exchange format for the materials community. Furthermore, while MatML has been designed for use in the industrial and research communities, the application also shows that it can support inquiry-based learning in a MIT materials science core undergraduate course.

Acknowledgements

MatDL is part of the National Science Digital Library project and is supported by National Science Foundation grant DUE-0333520 and National Institute of Standards and Technology grant 70NANB3H1079. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of NSF or NIST.

Notes

1. NSDL Materials Digital Library <http://matdl.org>.

2. PI: Laura M. Bartolo (College of Arts & Sciences, KSU); CoPIs: Sharon C. Glotzer (Materials Science and Engineering, U-M), Javed I. Khan (Computer Science, KSU), Adam C. Powell IV (Materials Science and Engineering, MIT), Donald R. Sadoway (Materials Science and Engineering, MIT); Senior Investigators: Kenneth M. Anderson (Computer Science, CU), James A. Warren, Deputy Director, and Vinod K. Tewary, Research Scientist (Materials Science and Engineering Laboratory, NIST).

3. The Accreditation Board for Engineering and Technology (ABET) with support from the Alfred P. Sloan Foundation convened a colloquy in San Diego, California on January 6-8, 2002. Fifty engineering educators, representing a range of institutions and disciplines, attended to determine "What are the fundamental objectives of engineering instructional laboratories?" independent of the method of delivery.

4. Document Object Model (DOM) is an interface that enables programs and scripts to dynamically access and change document content, structure, and style independent of platform or programming language. <http://www.w3.org/DOM/>.

5. Hypertext Preprocessor (PHP) is an open source, server-side, HTML embedded scripting language used to create dynamic Web pages. <http://www.php.net/>.

6. XML Path Language (XPath) is a language for addressing and fetching parts of an XML document. <http://www.w3.org/TR/xpath>.

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doi:10.1045/march2005-bartolo