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Materials Informatics: Facilitating the Integration of Data-Driven Materials Research with Education

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Materials informatics integrated into undergraduate and graduate materials education is a key component and critical issue to address the nation's shortage of well-trained, future scientists.

INTRODUCTION

The Materials Digital Library Pathway (*matdl.org*) currently serves as a pathway in the National Science Foundation-sponsored National Science Digital Library (NSDL) to facilitate the integration of materials research and education with a targeted audience of undergraduates and above.[1] The Materials Digital Library (MatDL) is a collaborative, distributive effort with an initial consortium including Kent State University, the National Institute of Standards and Technology, the Massachusetts Institute of Technology (MIT), the University of Michigan, Purdue University, and Iowa State University.

Materials informatics integrated into undergraduate and graduate materials education is a key component and critical issue to address the nation's shortage of well-trained, future scientists. Undergraduates utilizing networking technologies and informatics techniques in their research activities serve as early adopters of emergent cyberinfrastructure and as role models for future students. Their work demonstrates the potential of cyberinfrastructure-enabled scientific inquiry and learning.[2] Adhering to open standards and open access protocols,[3] MatDL leverages, implements, and maintains current, recognized, open-source collaborative software, such as code versioning systems, wikis, and content management systems to connect distributed teams, promote resource exchange, and facilitate information sharing.

THE NATIONAL SCIENCE DIGITAL LIBRARY

The National Science Digital Library provides a dynamic, organized point of access to science, technology, engineering, and mathematics (STEM) education and research resources targeted at all audience levels as well as access to services and tools that enhance the use of this content.[4] It includes ten pathways, each focused on a particular domain, such as biology, and audiences, such as middle school students. As part of the NSDL, the MatDL pathway serves the materials research and education community for undergraduates and above. The National Science Digital Library and MatDL comply with international standards and protocols, such as Dublin Core Metadata Standard (*http://dublincore.org/*) and Open Archives Initiative Protocol for Metadata Harvesting (OAI-PMH; *www.openarchives.org*) for interoperability, discovery, and accessibility.

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MatDL's Repository

The MatDL Repository, (*http://matdl.org/repository*) powered by Fedora/Fez, describes, stores, disseminates, and supports the repurposing of individual digital resources submitted by faculty, researchers, and students in the materials community, such as lecture notes and problems, *PowerPoint* presentations, images, and datasets. Fedora (*www.fedora-commons.org*) is an open-source Flexible, Extensible, Digital Object Repository Architecture that supports the reuse and re-purposing of individual digital resources.[5] Fez (*http://dev-repo.library.uq.edu.au/wiki*) is an open-source web front-end content management system for Fedora developed as part of the University of Queensland eScholarship Project and the Australian Partnership for Sustainable Repositories.

MatDL's MatForge

MatForge (*http://matforge.org*) currently provides on-line workspace for distributed government and university team-based, materials code projects using Subversion and Trac, to support coordinated code development efforts. Computational modeling plays a vital role in the development of advanced materials by enabling new or improved predictions of materials behavior. MatForge is a branded, trusted, non-commercial, and neutral site for open source code development in the materials community. By acting as a hub for computational materials code development, MatForge provides a workspace to support collaborative code development projects, hosting FiPy, which is affiliated with the National Institute of Standards and Technology, as well as the Department of Energy's Computational Materials Science Network, a consortium of 25 universities and government labs. In addition to providing integrated services for developers of

team-based materials code projects, MatForge helps to promote awareness and use of the codes in research and teaching, thereby facilitating the development of a pool of next-generation users in academe and industry.

MatDL's Soft Matter Wiki

Advances in cyberinfrastructure are revolutionizing the way people access and share information, transforming everything from the entertainment industry to social networks. However, the materials community has yet to take full advantage of these technologies for research, collaboration, and education. The Soft Matter Wiki (*http://matdl.org/matdlwiki*) explores the potential for current cyber technologies, including wikis and digital data repositories, for use in materials education. The Materials Digital Library Soft Matter Wiki and digital library repository developed at the University of Michigan in collaboration with Kent State University, is used in teaching concepts in soft materials and molecular simulation. These tools interface with classroom simulation modules developed using the Glotzilla simulation API (*http://matforge.org/glotzer*), providing students with a wide array of relevant-linked material ranging from definitions of key terms, explanations of algorithms, research examples, data, and links to relevant literature.

MatDL's Transport Phenomena Archive

The Transport Phenomena Archive (*http://teaching.matdl.org*) is an online space for collaborative development of educational resources related to the role of fluid flow, heat transfer, and mass transfer in the processing and performance of materials. The archive is currently home to over 100 such resources consisting of 661 files written by 30 authors, and includes homework problems, software, handouts, pedagogical materials (including Accreditation Board for Engineering and Technology [ABET] documentation) and readings. An international 14-member editorial board, comprising mostly materials science and engineering professors who teach transport, contribute toward the review of existing resources, as well as contribute new resources to the archive.

As part of the NSDL Materials Digital Library Pathway, all resources in the Transport Phenomena Archive are tagged with metadata in Dublin Core format and are available in the Fedora-based MatDL repository, supporting wide distribution across the NSDL and beyond. Homework problems include examples from all materials classes, including metals, ceramics, polymers, and electronic materials, as well as biological applications. They cover in varying levels of detail process sequences for given devices, such as the chain of integrated circuit fabrication from Czochralski crystal growth, to chemical and physical vapor deposition, to dopant diffusion and diffusion barrier formation.

MatDL's Virtual Labs

Virtual labs (*http://matdl.org/virtuallabs*) may provide a workable complement to physical labs, allowing students to achieve many ABET laboratory learning objectives while circumventing difficulties that make it impractical to offer physical labs to undergraduates. Virtual labs are being collaboratively developed initially at MIT, Carnegie Mellon University, and Kent State University by a design team with expertise in biophysics, chemistry, materials science, information science, and cognitive science. The goal of this effort is to use visualization and virtual laboratories to help students connect microscopic to macroscopic properties via learning resources based on recent and relevant research results that would work across discipline-specific courses (including chemistry, materials science, and biophysics).[6] This network of partners is working together to engage students in activity resembling and related to research to provide memorable context for attaching knowledge as well as to help students form mental models such as those experts employ to explain structure-property relationships.[7] To facilitate wide dissemination, the materials are integrated into MatDL as part of the NSDL. As a first step toward building community-focused dissemination, the MatDL Virtual Labs Wiki is publicly viewable where students, faculty, and other interested individuals can interact with all of the virtual labs, supplemental resources, and instructional materials from a single coherent site without downloading. Links to the online surveys, pre-tests, and post-tests are also available from the group-moderated wiki, making it as convenient as possible for interested students to provide valuable feedback about their virtual lab experience. The anticipated impact of this community-based effort is an open-access collection of vetted, reusable, and evolvable learning resources grounded in recent research results and suitable for a wide range of introductory science courses taught at 2-year and 4-year colleges.

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References

1. L.M. Bartolo et al., *Journal of Materials Education,* 28 (1) (2006), pp. 21–26.
2. National Science Foundation Cyberinfrastructure Council, "Cyberinfrastructure Vision for 21st Century Discovery," (NSF publication number 07-28). (Arlington, VA: National Science Foundation, 2007), *www.nsf.gov/pubs/2007/nsf0728/nsf0728.pdf* .
3. T. Hannay, "Web 2.0 in Science," *CTWatch Quarterly,* 3 (3) (August 2007), *www.ctwatch.org/quarterly/articles/2007/08/web-20-in-science/.*
4. L. Zia, "The NSF National Science, Technology, Engineering, and Mathematics Education Digital Library (NSDL) Program," *D-Lib Magazine,* 8 (11) (2002), *www.dlib.org/dlib/november02/zia/11zia.html.*
5. C. Lagoze et al., *International Journal on Digital Libraries,* 6 (2) (2006), pp. 124–138.
6. Boyer Commission on Educating Undergraduates in the Research University, "Reinventing Undergraduate Education: A Blueprint for America's Research Universities" (1998), *http://naples.cc.sunysb.edu/Pres/boyer.nsf/.*
7. A. Hunter, S. Laursen, and E. Seymour, *Science Education,* 91 (1) (2006), pp. 36–74.

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