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Data-Enabled Discovery and Design of Energy Materials (D^3EM): Structure of An Interdisciplinary Materials Design Graduate Program

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ABSTRACT

The Materials Genome Initiative (MGI) calls for the acceleration of the materials development cycle through the integration of experiments and simulations within a data-aware/enabling framework. To realize this vision, MGI recognizes the need for the creation of a new kind of workforce capable of creating and/or deploying advanced informatics tools and methods into the materials discovery/development cycle. An interdisciplinary team at Texas A&M seeks to address this challenge by creating an interdisciplinary program that goes beyond MGI in that it incorporates the discipline of engineering systems design as an essential component of the new accelerated materials development paradigm. The Data-Enabled Discovery and Development of Energy Materials (D^3EM) program seeks to create an interdisciplinary graduate program at the intersection of materials science, informatics, and design. In this paper, we describe the rationale for the creation of such a program, present the pedagogical model that forms the basis of the program, and describe some of the major elements of the program.

INTRODUCTION

Due to their importance as technology enablers, advanced materials are a critical component of the many technologies capable of solving overarching engineering/technical challenges that we currently face. On the other hand, the absence of materials with specific desired properties makes the deployment of potentially transformative technologies impossible. Unfortunately, the materials development cycle is often much slower than the timeframe over which technologies at the system level are developed. Recognizing this, the Office of Science and Technology Policy of the White House released the Materials Genome Initiative (MGI) in 2011 [1], which states the premise that the traditional materials development cycle—Edisonian in nature—is not the most optimal approach to address the lack of technology-enabling materials. Instead, the MGI proposes the synergistic combination of experiments and simulations within an informatics framework as a powerful strategy to accelerate the discovery and development of materials.

The aspirational goals espoused by the MGI require significant workforce development as the next generation of scientists/engineers should be able to create and deploy tools capable of connecting materials data to better-informed materials synthesis and computational analysis, and employ engineering design strategies for the goal-oriented development of materials. Unfortunately, current materials scientists—including those presently being trained at universities around the nation—often receive minimal training in data/information-related principles and methods. At the same time, students with informatics-related skills or familiar with concepts and methods of engineering systems design do not have the proper domain knowledge to apply their knowledge into materials discovery problems.

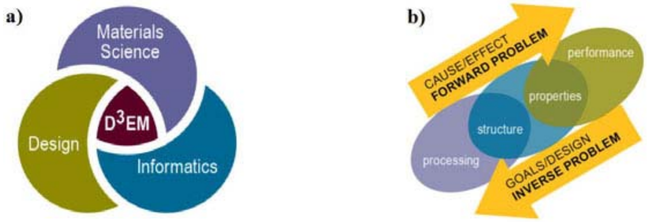

Figure 1. a) Data-Enabled Discovery and Development of Energy Materials (D^3EM) ; b) Forward and Inverse paradigms in materials science, adapted from Olson's work (reprinted with permission from AAAS [2]).

To address this gap, faculty belonging to the Colleges of Science and Engineering as well as the Center for Teaching Excellence at Texas A&M University (TAMU) designed a new interdisciplinary graduate program at the intersection of materials science, informatics, and design. The program, Data-Enabled Discovery and Design of Energy Materials, D^3EM (as figure 1a), is currently being funded by the National Science Foundation through their NSF Research Traineeship (NRT) Program. D^3EM was launched by faculty with expertise in materials science, informatics, engineering systems design, and STEM graduate education, with the main goal of creating an innovative program for educating trainees in this emerging interdisciplinary field. D^3EM is designed to provide the participating students with the skills necessary for creating and applying innovative data-enabled approaches with sound informatics and engineering design foundations to the discovery, design, and deployment of advanced materials, in particular those that enable the efficient and sustainable generation, storage, or utilization of energy.

In this work, we present the rationale for the disciplinary and interdisciplinary framework that informs the curriculum of D^3EM. Moreover, we provide a brief discussion of the pedagogical model used to achieve D^3EM's overarching goal to develop and institutionalize a new training model that produces scientists/engineers who are grounded in one discipline and have the professional and technical skills to effectively communicate within and collaborate and lead in interdisciplinary teams focused on materials development. Finally, we discuss some of the elements of the program, curriculum design, and the participation of both students and faculty in learning communities.

PEDAGOGICAL FRAMEWORK

Nearly two decades ago, Greg Olson proposed and popularized a framework (in figure 1b) that exploited the materials science paradigm of process-structure-property-performance (PSPP) relationships within an engineering systems framework in order to design materials [2]. Since then, traditional development of materials focuses on the so-called forward problem of determining material properties, given a structure (i.e., materials analysis) [3]. As such, this approach seeks answers to the question: 'given a set of material attributes (composition, phase constitution, microstructure), what are the corresponding properties and performance characteristics?' On the other hand, materials-by-design reverses this relationship. The problem is then one of synthesis, as the relevant question is: ‘given a set of performance requirements, what are the necessary material attributes and the required synthesis and processing routes to achieve those requirements.’

In order to frame the forward and inverse problems along the PSPP paradigm within the context of the curriculum of D^3EM, it is posited that the general disciplines of informatics and systems design can be aligned to this forward/inverse paradigm (figure 1b). Within the context of the PSPP paradigm, materials informatics can be seen as the collection of tools that enable the establishment of one-to-one relationships defined as the forward problem. On the other hand, systems design can be understood as the systematic search for a particular region within the PSPP domain that results in materials that meet specific performance goals subject to constraints, defined as the inverse problem. We thus consider the integration of materials science, informatics, and engineering systems design within a single interdisciplinary curriculum as the natural expression of the forward/inverse problem along PSPP relationships.

To create the envisioned interdisciplinary structure under the context of disciplinary Ph.D. programs, an interdisciplinary pedagogical model for the D^3EM program is needed. Based on sociocultural theory outlined by Vygotsky [4], learning is shaped not merely by the interaction between individuals, but also by cultural, historical, and social contexts/interaction. We structure aspects of the D^3EM program around four key educational concepts (mediated, relational, transformative, and situated learning [5]) which form the foundation of the D^3EM education model (figure 2).

Figure 2. D^3EM Pedagogical Model.

Sociocultural theory assumes that learning is established through social interaction; an indirect access to the world that is mediated by psychological and cultural tools, including language, mnemonic devices, and systems of counting. These tools shape the way individuals interact with the world. Given that academic disciplines frame the thinking and intellectual activity of individuals who use them, traditionally defined disciplines are considered an example of social relationships and practices. These practices mediate scientists’ and engineers’ approaches to solving a given problem. Becher [6] describes disciplines as self-regulating and self-sustaining communities that define their own identities by the sociocultural texts and methods of the discipline. Additionally, institutions have sets of social practices that guide participation in the community. In this context, the social practice of a discipline is transferred to students of that discipline through the program’s curriculum.

The acts of learning and cognition are social in nature, thus making them relational. That is, learning is socially constructed into a community of practice and interpersonal relationships are essential. Furthermore, given an emphasis on community of practice, learning should be situated into an activity. Interdisciplinary learning highlights this situated nature by placing individuals into varying contexts.

The creation of a new tool is part of the transformative process. Cultural tools facilitate actions, and change the way in which mental functions are structured. This study emphasizes transformation within the interdisciplinary context. This involves the "borrowing" of one discipline's theories, concepts, and methods to study a phenomenon that cannot be studied using the tools within the home discipline. Transformation happens when the tools are put to use.

DISCUSSION

The D^3EM program is supported by 17 faculty members from Materials Science Engineering, Engineering Design, Physics, Informatics, Chemistry, Mechanical Engineering, Chemical Engineering, Engineering Education, and Educational Psychology. Their commitment, engagement, and mentoring are crucial for students to develop professional and technical skills needed to engage in interdisciplinary research. The first cohort enrolled in the program, consisting of 6 Ph.D. students from Material Science Engineering, Chemical Engineering, Physics, and Chemistry, have completed the first-year. At least 41 funded graduate students and 40 additional participants will be recruited into the program throughout the five years. In the D^3EM Pedagogical Model (figure 2), program curriculum will mediate students' approaches to enhancing the discovery and design of energy materials. A Faculty Community of Scholars (FCS) and Student-led Learning Community will play significant roles in the relational and collaborative process among faculty and students. Additionally, Materials Design Studio will facilitate student's transformative learning to apply interdisciplinary concepts, theory, and methods in solving materials development problems. Lastly, the internship is a situated learning experience, offering access to real-word materials design and informatics problems.

<u>Curriculum</u>. During the first year of graduate studies, D^3EM students focus within their own disciplines to learn their discipline's preferred concepts, theories, methods, and forms of communication. After initial disciplinary grounding, students are expected to use their disciplinary knowledge and methods accurately and effectively.

In the second year, students are challenged by multidisciplinary courses, including Advanced Product Design, Materials Informatics, and Materials Science where they are first introduced to the concepts of disciplines outside of their own. To fill the gaps among disciplines, advisors and course instructors will employ the D^3EM competency rubrics to evaluate students' performance and provide supportive recommendations. Advisors identify strengths, gaps, and current level ability of students, providing recommendations to fill identified gaps such as courses, workshops, materials reading, and peer learning activities.

After completing multidisciplinary courses, students engage in activities (Materials Design Studio, ePortfolio) assigned to integrate concepts and tools drawn from individual disciplines and apply these towards complex challenging materials design problems. To facilitate situated learning, students are encouraged to take part in an internship to develop their interdisciplinary framework and practice their skills.

<u>Faculty Community of Scholars.</u> Faculty participate in a community of practice that facilitates the development of a shared interdisciplinary culture. The community formulates a greater appreciation of interdisciplinary issues, collaboration, and partnerships, as well as maintenance of a communication cadence between members. More importantly, this professional activity aligns faculty interests with the overall learning objectives of the program.

Reviewing the literature regarding interdisciplinarity helped us clarify the differences among the terms of multidisciplinary, interdisciplinary, and transdisciplinary, and learn the challenges of implementing interdisciplinary education and research. Each D^3EM curriculum has been reviewed, focusing on how to fill the disciplinary gaps when students are challenged by multidisciplinary and interdisciplinary courses. Given that some courses would not be offered by D^3EM faculty, outside faculty may be invited to participate in the FCS or a D^3EM faculty member may collaborate with the instructor, to ensure that program learning outcomes would be addressed.

To standardize assessment of program learning outcomes, professional skills, and technical skills 12 competency rubrics were developed: 1) interdisciplinary knowledge generation, 2) collaboration, 3) conflict resolution, 4) oral communication, 5) written communication, 6) self-reflection, 7) ethics, 8) interdisciplinary research, 9) multidisciplinary skills, 10) materials science engineering, 11) informatics, and 12) design. Rubrics are helpful to identify student's current ability. Based on assessment results, advisors could provide feedback and recommendations to students.

In addition to learning performance, the mentoring process also covers areas such as the student's research progress, skill development, career development, wellness, and goal planning. An individual development plan (IDP) template was created to help structure mentorship interactions and goals. The IDP is a method for students to develop an action plan for the upcoming year with the help and input of their advisor and mentors. In order to facilitate engagement in self-reflection and improve writing skills, an ePortfolio template and related assignments are incorporated..

Student-led Learning Community. The student-lead Learning Community also plays a significant role in the relational process among students. Students are encouraged to form interpersonal relationships with their peers outside of their discipline. This biweekly meeting assists students in the development of leadership, communication, interdisciplinary, and self-reflection skills. Similar to the FCS, each session has prepared goals and topics in advance. These topics align with the program learning outcomes developed by faculty as goals for a student participating in the program. To enhance interdisciplinary learning, several skills are developed including critical thinking, interdisciplinary communication, ethical behavior, interdisciplinary collaboration, and organization/management skills.

Initial student sessions included a review of the expectations of the program: learning outcomes, competency rubrics, IDP, and ePortfolio.. Peers taught an area of their research within their discipline and then opened to interdisciplinary discussion regarding how components of the discipline described could support gaps in their respective disciplines. Invited speakers focused on interdisciplinary conflict management and ethical behavior with ensuing discussion bringing the experience to current concerns and situations as a learning experience.

Materials Design Studio. To emphasize experiential, problem-based learning and prepare students for the next stage of their careers as they begin to establish the direction of their research, a Materials Design Studio was created. This course facilitates the transformative process. Students in interdisciplinary teams will work on real-world materials problems defined by industrial and governmental partners in consultation with D^3EM faculty, or linked to existing interdisciplinary research at TAMU. The goal is to solve materials development problems by combining computational/experimental approaches, and by using design theories as well as informatics approaches.

Internships. Students will enrich their D^3EM trainee experience by engaging in a situated learning experience involving real-world materials design and informatics problems with societal value through industry or government lab internships. A written reflection regarding the internship will be required in the integrated learning portfolio. These experiences will contribute significantly to the trainees' professional development, providing meaningful skills, a broader perspective on socially and commercially relevant research, and enhanced networking opportunities.

PROGRAM OUTLOOK

The structure of an interdisciplinary graduate program is built upon the three-legged foundation of Materials Science, Engineering Design, and Informatics, and designed to train students to face increasingly complex Materials Engineering challenges. Due to the interdisciplinary nature of the project, we have encountered mixed perspectives from both faculty and student participants. At the outset, participants expressed a diverse set of expectations of themselves and others. Initial differences made communication difficult, however due to the relational process we were able to improve interdisciplinary communication over the course of the first year. The FCS provided a critical outlet for information exchange, which permitted faculty to speak freely about topics outside of their discipline without judgement. Overall, the Student-led Learning Community and FCS increased participant interactions, furthered collaborations, and enhanced relationships.

The impact of each of the program components (curriculum, learning community, IDP, ePortfolio, design studio, and internship) on program learning outcomes, professional skills, and technical skills will be assessed. First, however, the competency rubrics will undergo a thorough validity study to ensure they are measuring what is intended as they serve as a key component of the assessment of student learning in the program. We hope other institutions will benefit from our studies and experiences as they design future interdisciplinary programs. Finally, initial observations suggest an internal debate in students regarding identity; students struggled to combine their interdisciplinary work with their disciplinary work with varying degrees of success. This internal struggle will be further explored in future work.

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