The University Senate of Michigan Technological University
Proposal 14-21

(Voting Units: Academic)

Establishment of a New Graduate Certificate in Computational Materials Science

Submitted by: Department of Materials Science & Engineering

1. **Proposal Date:**
   June 3, 2020; revised December 10, 2020

2. **Proposing Contacts and Department:**
   Douglas Swenson, Materials Science and Engineering
   Yu Wang, Materials Science and Engineering

3. **Sponsor Department Approvals**
   Materials Science and Engineering

4. **General Description and Characteristics of Program:**

4.1 General Description of Certificate

The Certificate in Computational Materials Science is a ten credit program of 2 required and two electives designed to provide a fundamental knowledge of computational materials science. The program of study provides basic understanding of the physical principles and practical skills to perform computational materials research. Recipients of this certificate will be able to apply computational thermodynamic and kinetic principles, numerical algorithms, and computer programming to simulate the materials processes required to develop specific materials microstructures and properties and study the processing-microstructure-property relationships. This certificate would be of interest to engineers/students involved/interested in development and design of materials. The certificate will be offered on campus and can be earned fully on-line.

4.2 Catalog Description

The Certificate in Computational Materials Science is designed to develop skills and competencies in computer modeling and simulation of microstructural evolution and property change during materials processes, including computational principles, numerical algorithms, and programming implementation of thermodynamics of materials science, kinetics of microstructure development, and microstructure-property relationships. In addition, the curriculum integrates building skills in communication, project development, and literature review from real-world problems.

5. **Rationale for Certificate:**

The rationale for this certificate can be found in the *Materials Genome Initiative for Global Competitiveness* (Office of Science and Technology Policy, White House), which highlights the national interest in computational materials science field. Computational materials science has become a major branch of materials research, complementary to experimental and theoretical studies. It plays an indispensable role in academia and has become increasingly important for

industry. The proposed courses within this certificate are offered on-line, as well as face-to-face, such that engineers and scientist in the field or related fields may earn the certificate.

6. Related Programs:

There are very few graduate certificate programs in computational materials science. The most closely related program is at Boise State:

https://www.boisestate.edu/graduatecatalog/programs/graduate-certificate-in-computational-materials-science-and-engineering/

This is a 9-credit interdisciplinary certificate which applies computational tools in the field of materials science and engineering. Topics covered are first-principles techniques, molecular simulation, supercomputing, big data analysis, and scientific algorithm development.

There are other programs where computational materials science is part of master's degree, such as Northwestern:

https://www.mccormick.northwestern.edu/materials-science/documents/ICME_Brochure%202-2-18.pdf

And there are programs for undergraduates, such as the program at Illinois:

https://cse.illinois.edu/files/2018/04/MSE_certificate.pdf

7. Projected Enrollments:

We anticipate significant enrollment from both MSE's on-campus and distance MS and PhD graduate students, plus students from related fields that have an interest in the materials side of their discipline. Interest from students enrolled in peer graduate programs seeking transferrable coursework is also anticipated.

Semester	On-campus Enrollment	On-line Enrollment
Fall 2021	3	5
Fall 2022	5	5
Fall 2023	5	5
Fall 2024	5	5
Fall 2025	5	5

8. Scheduling Plans:

No change in the regular scheduling of the existing courses is anticipated. The departments delivering the online courses have agreed to fit them into their regular scheduling plans.

9. Curriculum Design: Max three of ten certificate credits may be 3000 or 4000 level.

Required Coursework (4 credits):

- MSE 5540 Advanced Computational Materials Science and Engineering **OR**
  MSE 4540 Computational Materials Science and Engineering (both 3 cr., students are disallowed from receiving credit for both)
- MSE5970 - Special Topics - Graduate Materials Science and Engineering,
  1 cr. Topic: Perspectives on Computational Materials Science;
  Restrictions: Permission of the Department

(permission will be granted in the student's last semester of the certificate)

Elective Coursework (6 credits) (only 3 credits at 4000 level, 0 credits at 4000 level if MSE 4540 is taken)

- MSE 5140 Mechanical Behavior of Materials
- MSE/PH 5151 Quantum Optical Materials
- MA 4620 Numerical Methods for PDEs
- MEEM 4405 Introduction to Finite Element Method

  OR BE 5115 Finite Element Modeling with Biomedical Applications

  OR CEE5202 Finite Element Analysis

Course Descriptions:

MSE 4540 - Computational Materials Science: Theory, Modeling, Simulation, and Practice
Theories of materials science from first principles to constitutive laws. Materials modeling and computer simulation at multiple length and time scales. Laboratory practice of various computational methods.
Credits: 3.0
Lec-Rec-Lab: (2-0-3)
Semesters Offered: Fall
Restrictions: May not be enrolled in one of the following Class(es): Freshman, Sophomore

MSE 5540 - Advanced Computational Materials Science: Theory, Modeling, Simulation, and Practice
Theories of materials science from list principles to constitutive laws. Materials modeling and computer simulation at multiple length and time scales. Laboratory practice of various computational methods.
Credits: 3.0
Lec-Rec-Lab: (2-0-3)
Semesters Offered: Fall
Restrictions: Must be enrolled in one of the following Level(s): Graduate

MSE 5970 - Special Topics - Graduate Materials Science and Engineering
Special Topics in Materials Science and Engineering at the Graduate level. Credits: variable to 4.0; Repeatable to a Max of 8
Semesters Offered: Fall, Spring, Summer
Restrictions: Permission of instructor required; Must be enrolled in one of the following Level(s): Graduate

PH 5151 / MSE5151- Quantum Field Theory for Photonics and Materials
This course will review the basics of quantum mechanics and second quantization, and cover quantum field theoretical methods, including Wick's theorem and Feynman diagram techniques, for absolute zero and non-zero temperatures (Matsubara frequencies) and their application in photonics, properties of materials and condensed matter physics.
Credits: 2.0; Graded Pass/Fail Only
Lec-Rec-Lab: (2-0-0)
Semesters Offered: Spring - Offered alternate years beginning with the 2020- 2021 academic year
Pre-Requisite(s): PH 3410 and PH 3411(C)

PH 4390 - Computational Methods in Physics
An overview of numerical and computer methods to analyze and visualize physics problems in mechanics, electromagnetism, and quantum mechanics. Utility and potential pitfalls of these methods, basic concepts of programming, UNIX computing environment, system libraries and computer graphics are included.
Credits: 3.0
Lec-Rec-Lab: (2-0-3)
Semesters Offered: Fall

Pre-Requisite(s): PH 2020 and PH 3410

MEEM 4405 - Intro to the Finite Element Method
Introduces the use of the finite element method in stress analysis and heat transfer. Emphasizes the modeling assumptions associated with different elements and uses the computer to solve many different types of stress analysis problems, including thermal stress analysis and introductory nonlinear analysis.
Credits: 3.0
Lec-Rec-Lab: (0-2-2)
Semesters Offered: Fall, Spring, Summer
Pre-Requisite(s): MEEM 3400 and (MA 2320 or MA 2321 or MA 2330) and (MA 3520 or MA 3521 or MA 3530 or MA 3560)

BE 5115 - Finite Element Modeling
The course teaches both fundamentals of finite element theory and hands-on experience for bio-engineers.
Credits: 3.0
Lec-Rec-Lab: (3-0-0)
Semesters Offered: Spring
Restrictions: Must be enrolled in one of the following Level(s): Graduate

CEE 5202 - Finite Element Analysis
Introduction to the use of finite element methods in structural analysis. Covers the finite element formulation, 1- and 2-D elements, including isoparametric elements, axisymmetric analysis, plate and shell elements, dynamics, buckling, and nonlinear analysis.
Credits: 3.0
Lec-Rec-Lab: (0-3-0)
Semesters Offered: Spring Pre-Requisite(s): CE 4201 or CEE 4201

MA 4620 - Numerical Methods for PDEs
Derivation, analysis, and implementation of numerical methods for partial differential equations; applications to fluid mechanics, elasticity, heat conduction, acoustics, or electromagnetism.
Credits: 3.0
Lec-Rec-Lab: (0-3-0)
Semesters Offered: Fall
Pre-Requisite(s): (MA 3520 or MA 3521 or MA 3530 or MA 3560) and MA 3160

9. Model Schedule Demonstrating Completion Time

The certificate is designed to be completed in 1 or 2 semesters. A 2-semester schedule with a fall start is shown.

Fall Semester
- MSE5540 Computational Materials Science and Engineering
- Pick 0 or 1 courses from the following:
  - MSE5140 Mechanical Behavior of Materials
  - MEEM 4405 Introduction to Finite Element Method
  - MA4620 Numerical Methods for PDEs

Spring Semester (MSE5540 or MSE4540 taken in fall)
- MSE 5970 Special Topics- Perspectives on Computational Materials Science
- Pick 1 or 2 courses
  - PH 5151 Quantum Optical Materials
  - BE 5115 Finite Element Modeling with Biomedical Applications

10. Library and other Learning Resources

No library or other learning resources are required at this time.

11. **Faculty Resumes**
The following MSE faculty will be supporting the program.
Prof. Yu Wang
Prof. Yongmei Jin
Prof. Miguel Levy

12. Equipment
No additional equipment will be required.

13. **Program Costs**
Initial costs for offering the certificate will not incur additional costs. As online/remote instruction enrollment grows, the additional costs associated with instruction will be covered from tuition return from the students who are enrolled online.

14. Space
There are no new space requirements.

15. **Policies, Regulations, and Rules**
Not applicable

16. Accreditation Requirements
Michigan Tech is accredited by the Higher Learning Commission (HLC). The proposed certificate will meet HLC criteria 3 and 4. The proposed certificate will not seek additional accreditation.

17. Planned Implementation Date
Fall 2021

18. **Assessment**

Upon completion of the Computational Materials Science Graduate Certificate, students will:

1. be able compare/contrast the leading methods and approaches utilized to computationally simulate material behavior and response.
2. be able to simulate material behavior and response using at least three appropriate computational approaches and tools

Approval Process
Departmental Graduate Committee May 29, 2020
Department: May 29, 2020; revised December 10,2020
College of Engineering: June 9, 2020
Graduate School: June 17, 2020
Provost's Office and Deans' Council: June 23, 2020
Approved by the Senate:
Approved by the President: