TO: The Engineering Faculty

FROM: The Faculty of the School of Materials Engineering

RE: New graduate course – MSE 57000 Introduction to Materials Modeling and Informatics

The Faculty of the School of Materials Engineering has approved the following new graduate course in Sept. 2022 (see attached document for course description). This action is now submitted to the Engineering Faculty with a recommendation for approval.

FROM:
MSE 59700: Modeling & Simulation for Materials, Sem. 1, 2, SS, Class 3, Cr. 3. MSE 27000 and MSE 37000 or graduate standing
Temporary course number. Course was taught Spring 22, 20, 19, and 17. Enrollments were 19, 13, 14, and 6.

TO:
MSE 57000 Introduction to Materials Modeling and Informatics Sem. 1, 2, SS, Class 3, Cr. 3. Prerequisites: MSE 27000 and MSE 37000 or graduate standing

This course provides an introduction at the graduate level to theory and methods for simulating the structure and properties of materials. The course will provide a broad initial overview of many atomistic modeling techniques, followed by a detailed study of density functional theory (DFT) over several weeks, then a few lectures on classical molecular dynamics (MD) and Monte Carlo (MC) simulations, and finishing with an introduction to materials informatics techniques which rely on learning from materials data. Students will obtain an essential understanding of quantum and classical theory and become acquainted with practical methods for running DFT, MD and MC simulations, as well as combining such simulations with simple machine learning and data science methods for materials design. Existing and new tools on nanoHUB, access to open-source simulation software, and writing simple Python code will be utilized for all necessary coursework and exercises. Permission of department required.

Reason: This course has been taught successfully as a temporary course and seen steady growth in enrollment. It is now being submitted for a permanent course number. It is expected that in the future the course may also be delivered via distance education using a lecture capture mode in the future.

David Bahr
Head of MSE

Proposal for New Graduate Level Course for Academic Review
MSE 57000 – Introduction to Materials Modeling and Informatics

Note: The detailed course proposal is intended for academic review by the appropriate area committee of the Graduate Council. It supplements the Form 40G that is intended for administrative review of the Graduate School and Registrar.

TO: Purdue University Graduate Council

FROM: Faculty Member: Arun Mannodi Kanakkithodi
Department: School of Materials Engineering
Campus: West Lafayette

DATE: March 25, 2022

SUBJECT: Proposal for New Graduate Course

MSE 57000 Introduction to Materials Modeling and Informatics
2 lectures per week (Tue, Thu), 75 minutes each

1. Course Description

This course provides an introduction at the graduate level to theory and methods for simulating the structure and properties of materials. The course will provide a broad initial overview of many atomistic modeling techniques including ab-initio, classical molecular dynamics (MD) and Monte Carlo (MC) simulations, followed by a detailed examination of density functional theory (DFT) over several weeks, transitioning on to high-throughput computations and dealing with materials datasets, and finishing with an introduction to materials informatics techniques and a few lectures on training and deploying machine learning models for materials design. Students will obtain an essential understanding of quantum and classical theory and become acquainted with practical methods for running DFT simulations, as well as combining such simulations with simple machine learning and data science methods for accelerated materials design. Existing and new tools on nanoHUB, access to open-source simulation software, and writing simple Python code will be utilized for all necessary coursework and exercises.

2. Justification for the Course

2.1 Justification of the need for the course

This course is designed for senior undergraduate students and graduate students from Materials, Mechanical, or Chemical engineering departments who are interested to learn how different types of materials (metals, alloys, ceramics, polymers, molecules) and different types of properties (elastic, electronic, magnetic, optical, thermal) could be modeled using quantum mechanics and methods rooted in data science. The course material will complement the topics covered in various other courses such as MSE 270 (atomistic materials science), MSE 370 (electrical, optical and magnetic properties), MSE 597 (solid state materials), and MSE 697 (atomistic view of materials). Currently, there is no permanent materials engineering course that

provides basic expertise in modeling and informatics to students who are new to research and looking to get started in computational materials science or bolster their overall research skillset with theoretical and data-based approaches. A version of this course has been taught by instructor Mannodi Kanakkithodi two times: in spring 2021 for a class of 11 students, and in spring 2022 for a class of 19 students, both offerings leading to overwhelmingly positive feedback from undergrad and grad students alike. Furthermore, the proposed course is distinct from the grad course MSE 697 in terms of providing a more general overview of materials modeling and an appropriate complexity of course material for undergrads and beginner grads, focusing a lot on materials data, ML, and screening, and proving as a preliminary / introductory offering for grad students who can go on to take MSE 697 and majorly apply modeling and informatics in their thesis projects.

2.2 Justification that course will be taught at a graduate level

MSE 57000 will be taught at the graduate level. The course builds on some undergraduate topics (MSE 270, 370) and will be complementary to some graduate courses (MSE 597 Solid State Materials and MSE 697). Students taking this course will be expected to have a basic background of differential equations, the structure of materials, electronic and mechanical properties, and phase transformations of materials. The course material will cover materials modeling textbooks by D.S. Sholl (2009), F. Giustino (2014) and D. Frenkel (2002), the machine learning textbook by C.M. Bishop (2006), as well as several peer-reviewed journal articles reviewing modeling and informatics techniques.

2.3 Justification for online delivery

This course may of interest to many students pursuing distance learning or online Masters degrees in engineering disciplines. An essential knowledge of the concepts and practical tools in computational materials science is needed for all graduates performing materials research.

3. Learning Outcomes and Methods of Assessment

3.1 Learning Outcomes

By the end of the course, students are expected to be able to (a) design, execute and analyze simple simulations using techniques appropriate for the problem at hand, (b) recognize the approximations and level of accuracy associated with each modeling technique, iii) establish a foundation for exploring materials modeling techniques in greater depth and applying them to their own research projects, and (d) recognize the importance of machine learning and data science, and identify when to apply such techniques for materials datasets.

3.2 Assessment Methods

Assessment will be achieved in three different ways: regular quizzes (one roughly every 3 lectures) with multiple-choice questions to evaluate basic understanding of lecture material, homework assignments (one roughly every 5-6 lectures) that ask students to conceptualize, execute, and analyze in-depth materials simulations using readily available resources, and one final group project where students will be assigned a research problem and asked to solve it

using the techniques covered in class. Students will be strongly encouraged to attend and engage during lectures and office hours (which will be scheduled weekly). Grading of assignments and research projects will be based on how well a student understands the problem, how effectively the simulations are deployed, and how well the solutions have been explained in terms of materials chemistry and physics and in the context of similar results from the literature.

3.3 Final Grading Criteria

Grading will be based on a fixed scale that is familiar to advanced undergraduate and first and second year graduate students. The breakdown will be:

Quizzes: 40 %
Homework: 45 %
Final Project: 15 %

Final grades may be adjusted depending on class performance on project and HW assignments. The following grading scale will be used (based on numerical scores assigned for all quizzes, HW, and projects, converted to a 100-point scale):
> 95% → A+
90% - 95% → A
85% - 90% → B+
80% - 85% → B
75% - 80% → C+
70% - 75% → C
65% - 70% → D+
60% - 65% → D

3.4 Methods of Instruction

Lecture – In-class lectures, and if necessary pre-recorded lectures, will be used to help the students to achieve the learning outcomes. This will include basic overview of all concepts via slides and blackboard writing, as well as demonstrations of state-of-the-art applications of relevant research methods for problem solving in the literature.

3.5 Prerequisite(s)

Graduate Standing OR MSE 270 and MSE 370.

4. Course Instructor

Arun Mannodi Kanakkithodi, Assistant Professor MSE:

Prof. Mannodi Kanakkithodi has years of experience and training in materials modeling and informatics techniques for the efficient design of new materials for a variety of energy applications. He has taught the proposed course as an elective to a group of 30 graduate and undergraduate students over the last two spring semesters and received positive reviews and interest from students for follow-up research projects. He has also previously designed and

organized data science and materials modeling-related lectures, tutorials and course material for the Materials Research Society and nanoHUB.

5. Course Outline:

- Introduction to Materials Modeling: Methods and Successes (1 week / 2 lectures)
- Brief review of Statistical Mechanics, Molecular Dynamics, and Monte Carlo Simulations (3 weeks / 6 lectures)
- Brief Review of Quantum Chemistry (1 week / 2 lectures)
- Density Functional Theory (7 weeks / 14 lectures)
- Materials Data: High-Throughput, Screening, and Databases (2 weeks / 4 lectures)
- Machine Learning in Materials Science (2 weeks / 4 lectures)

6. Reading List

The following books and review papers are recommended reading. Course material will derive from each source. Other reading material, especially published journal articles, will be provided during the course. Students are not expected or required to purchase any books, but pdfs of multiple textbooks listed below are freely available online. The lecture slides, notes, and recommended journal articles (which will be available online using Purdue libraries) will be sufficient for learning the course material. Reading material will reside on Brightspace.

- D. S. Sholl and J. A. Steckel, "Density Functional Theory: A Practical Introduction", John Wiley & Sons, Inc., 2009.
- D. Frenkel and B. Smit, "Understanding Molecular Simulation: From Algorithms to Applications", Academic Press, 2002.
- R. M. Martin, "Electronic Structure: Basic Theory and Practical Methods", Cambridge University Press, Cambridge, UK, 2004.
- F. Giustino, "Materials Modelling using Density Functional Theory", Oxford University Press, Oxford, UK 2014.
- J. Neugebauer and T. Hickel, "Density Functional Theory in Materials Science", Comput. Mol. Sci. 3: 438–448 (2013).
- A.D. Becke, "Perspective: Fifty years of density-functional theory in chemical physics", J. Chem. Phys. 140, 18A, 301 (2014).
- J. Schmidt et al., "Recent advances and applications of machine learning in solid-state materials science", npj Comput. Mater. 5, 83 (2019).
- K. T. Butler et al., "Machine learning for molecular and materials science.", Nature. 559, 547–555 (2018).
- L. Ward et al., "Matminer: An open source toolkit for materials data mining", Comput. Mater. Sci. 152, 60-69 (2018).

7. Past Course Syllabus Example

MSE 59700: Modeling & Simulation for Materials

Spring Semester, 2022

Lectures
Tuesday & Thursday, 10:30am-11:45am, PHYS 111

Instructor
Prof. Arun Kumar Mannodi Kanakkithodi
Office: DLR 103F
Email: *amannodi@purdue.edu*

Course description
Students will be introduced to the fundamental concepts behind the electronic and atomic structure description of materials. They will learn to apply materials modeling techniques, ranging from first principles simulations to force field-based molecular dynamics to machine learning-based methods. In-person and online lectures, regular quizzes and homework assignments, and critical reading of published literature will be utilized in this course. By the end of the course, students are expected to be able to (a) design, execute and analyze simple simulations using techniques appropriate for the problem at hand, (b) recognize the approximations and level of accuracy associated with each modeling technique, and iii) establish a foundation for exploring materials modeling techniques in greater depth and applying them to their own research projects.

Topics
Introduction to Materials Modeling: Methods and Successes
Brief Review of Quantum Chemistry
Density Functional Theory
Review of Statistical Mechanics
Molecular Dynamics Simulations
Monte Carlo Simulations
Machine Learning in Materials Science

Textbook
There is no single textbook that covers all the topics that will be taught in this course. Lecture notes/slides, homework assignments, and announcements will be available on Brightspace: *https://purdue.brightspace.com/d2l/login*.
Additional reading material will include selected chapters of books and recent literature.
Online lectures presented by Prof. Alejandro Strachan on electronic structure & bonding are available via nanoHUB: *https://nanohub.org/courses/FATM*

Course organization
The class will meet for 2 lectures per week, each lecture being 75 minutes long (10.30 am – 11.45 am). Homework assignments will be provided periodically (typically every 1-2 weeks). Assignments will require online simulations (using the nanoHUB platform) or some basic coding (using Python). Students need to set up and run their own simulations. Homework must be submitted by due date. Short quizzes will be given in class (roughly every week) to evaluate

student progress. Office hours will be scheduled for 1-2 hours every week, and students are encouraged to reach out to the instructor via email any time.

Grading Policy
Homework Assignments: 50%
Quizzes: 50%

Prerequisites

Students should have working knowledge of college-level physics and math, and access to a working computer. Basic programing in Python will be needed to complete some homework assignments.