Introduction

This guide describes the policies and procedures for the Materials Science and Engineering doctoral program (https://nano.nd.edu/materials-science/) at the University of Notre Dame. In this interdisciplinary program graduate students are also expected to adhere to the guide for their home departments:

- Department of Aerospace & Mechanical Engineering Graduate Studies Handbook
- Department of Chemistry and Biochemistry Guide to Graduate Studies
- Department of Chemical and Biomolecular Engineering Guide to Graduate Studies
- Department of Civil & Environmental Engineering and Earth Sciences Graduate Handbook
- Electrical Engineering Department Graduate Studies Handbook
- Department of Physics Guide for Graduate Students

The Graduate School policies regarding degree progress and requirements to maintain eligibility for financial support and health care subsidies are contained in the Du Lac, the University’s student policy and procedure manual, and the Graduate and Professional Student Handbook. Nothing herein is to be interpreted as contrary to the regulations of the Graduate School.

This program guide provides the official policies of the degree program. Any deviation from these policies requires the written approval from the program Steering Committee which will then document the exception in the student’s permanent file. Deviations will be considered on a case-by-case basis; an exception in a particular case will not imply a change in policy.

For questions regarding the graduate program please contact Derek Lake, NDNano Associate Director, 206 Cushing Hall, email: dlake@nd.edu, or the program director, Professor Alan Seabaugh 230A Fitzpatrick Hall, aseabaug@nd.edu.

BASIC RESPONSIBILITIES OF STUDENTS

Registration & Enrollment

A graduate student must meet the home department requirements to be full time as explained in the home department’s graduate studies guide. This includes registration and enrollment, both responsibilities of the student.

Satisfactory Degree Progress
Students must be making satisfactory progress toward their degree and remain in good standing in accordance with their home department’s policies. This includes but is not limited to completion of qualifying exams, successful candidacy exam review, dissertation completion and defense, etc. The exact degree milestones will be detailed in the home department graduate studies guide.

**Grades**
The most readily used means for assessment of the student's academic progress is through grades assigned in course work. The Graduate School grading system is on a four-point basis. Grades recorded for graduate courses are: A (4.0), A- (3.667), B+ (3.333), B (3.0), B- (2.667), C+ (2.333) and C (2.0). Students must meet the minimum GPA requirements for their home department.

**Teaching and Research Responsibilities**
Most graduate students are supported by research grants and contracts. Each student is responsible for meeting the requirements of his/her research position, which should be considered a full-time position. Students should be on campus and meet with their research supervisor regularly.

Most departments in the Colleges of Engineering and Science require their graduate students to assist with teaching. The director of graduate studies in the student’s home department may assign teaching assistant duties according to the policies of the department.

**Holidays and Time-off**
The policies for holidays and time-off for the home department should be followed.

**Office and Laboratory Facilities**
Each home department supports office space and individual research laboratories. Students are responsible for acquainting themselves with and following the proper safety procedures for the laboratories they use. Because the offices and laboratories are diverse in their purposes, procedures, and equipment, specific safety procedures are not listed here. However, all users of these offices and laboratories are to observe the following general safety and security procedures:

1. A student may be issued keys or electronic access to university buildings. Keys may not be traded among, loaned to, or passed on to other students and must be returned as soon as the need for regular access has passed.
2. Laboratory users share in maintaining its security and cleanliness. Laboratory doors are not to be propped open or left unlocked when the laboratory is unattended, and must be locked at the end of the working day.
3. Unauthorized users are not allowed into a laboratory.
4. Guests may be invited into a laboratory, but may not be left unsupervised. The home department is responsible for the guests' safety.
Safety
Office facilities and laboratory spaces have an integrated safety plan. Each student should be familiar with it, and each advisor or his/her designee should instruct students in laboratory safety. Each student should bring to the attention of the laboratory supervisor or advisor any unsafe laboratory situations they encounter. If a student does not feel that a concern has been adequately addressed, that student should contact the program director. The following general rules apply to all laboratories:

1. Students must complete assigned training through ComplyND before working in laboratory facilities.
2. Each student using a laboratory must be acquainted with all the particular safety procedures and safety equipment in the laboratory. These include the locations of emergency controls and the locations and use of all safety equipment and first aid supplies.
3. Students should contact their advisor or other laboratory management if they see an unsafe situation, or feel the need for additional or different personal protective equipment.
4. Graduate students who supervise undergraduate laboratories assume primary responsibility for safety procedures. If additional safety supplies (such as hard hats or safety glasses) are required, the course instructor should be notified.
5. Any graduate student developing a new experiment or acquiring new equipment will also be responsible for developing and recording the proper safety procedures associated with the new equipment.
6. Observed inadequacy of laboratory safety procedures or equipment must be reported immediately to a faculty member so that the situation may be corrected.
7. Violations of safety procedures or the creation of unsafe or unhealthy conditions must be reported to the responsible faculty. Failure to work safely or to maintain orderly, professional working environments will result in the forfeiture of all office or laboratory privileges.

In addition to the safety policies outlined here, students should review and understand the home department’s safety policies.

Leaves or Study at Other Sites
Students should review their home department policies around leaves and study at other sites.

III. Program Structure

The Materials Science and Engineering doctoral program is administered by the Center for Nano Science and Technology (NDnano) and is housed across participating departments in the
Colleges of Engineering and Science. The program is a Ph.D. program, and the Graduate School does not grant an M.S. degree in Materials Science and Engineering.

Administration
All policy-making and administrative authority in the Materials Science and Engineering doctoral program resides with the Steering Committee and the program director. Any policy question or administrative matter should be referred in writing to the Steering Committee via Heidi Deethardt, 206 Cushing Hall, MSE-list@nd.edu. Matters that cannot be resolved satisfactorily can be appealed to the Graduate School, via the Dean of the Graduate School. The program director is Professor Alan Seabaugh, 230A Fitzpatrick Hall, aseabaug@nd.edu.

Home Department
Each student in the program will belong to a home department. The home department is the department where the student was admitted. The home department in conjunction with the advisor will provide office and laboratory facilities for the student. The student is required to fulfill any teaching assistant, service, and professional development requirements as other Ph.D. students in the home department.

Financial Support
Most full-time students receive a stipend. Funds for these stipends typically come from externally funded grants and contracts of the student's advisor. One-year Materials Science and Engineering Fellowships are available and awarded annually by the Executive Committee.

Materials Science and Engineering Fellowships
Materials Science and Engineering Fellowships will be awarded each year by the Executive Committee. The Fellowship is for one-year and is non-renewable. The application process is joint between the student and the student’s advisor. The following items are required when applying for a fellowship: 1) A two-page research proposal written by the faculty advisor, 2) a one-page statement of interest from the student, 3) and the student’s curriculum vitae. The Materials Science and Engineering Fellowships will typically be used in the student’s second or third years of study. Preference for these fellowships will be given to students with co-advisors across disciplines. Each student may only be awarded the Materials Science and Engineering Fellowship one time. A student does not have to be awarded a Materials Science and Engineering fellowship to participate in the Materials Science and Engineering graduate program.

IV. Advising
One of the most important matters for graduate students is the choice of a faculty advisor. This choice can have a great effect on the student’s time in graduate school and long-term career path. Students in this program should follow their home department policies to select a graduate research advisor. Students are required to have a co-advisor that crosses disciplines
and encouraged to be from outside the department. Students should work with their primary research advisor to select a co-advisor within the policies laid out by their home department. Exceptions to having a co-advisor have to be approved by the Steering Committee.

**Examination Committee**
Each student should follow the home department guidelines for the selection of his/her examination committee. The student’s co-advisor should be part of the examination committee.

**Professional Development and Career Planning**
The Graduate Career Center resources are focused on graduate student success - helping each student to be the best prepared in order to obtain strong career outcomes after his/her time at Notre Dame. All Materials Science and Engineering students should meet any requirements with respect to the Graduate Career Center as stated in the home department’s policies. The Center is located in the Graduate School, 110 Bond Hall, and online at [http://gradcareers.nd.edu/](http://gradcareers.nd.edu/).

**Course Requirements**
Materials Science and Engineering students reside in a home department and are expected to meet the course requirements of the home department. Students will take a minimum of nine credit hours from a designated set of Materials Science and Engineering graduate courses (Appendix D). The courses will be taken in addition to course requirements of the home department or as electives within the course requirements as dictated by the home department policies. The Steering Committee will make the final decisions on accepting graduate course credits earned outside of Notre Dame towards the Materials Science and Engineering doctoral program. The Academic Committee will make decisions on the addition or removal of courses on the list of approved Materials Science and Engineering graduate courses.

**Degree Program**
The Materials Science and Engineering graduate student must meet the requirements of that student’s home department. In addition, this student must have a doctoral thesis that has a significant materials component. The Materials Science and Engineering student should submit the following to the Steering Committee to have his/her thesis approved for the Materials Science and Engineering Program: 1) a letter to the Steering Committee explaining how the thesis advances the understanding of materials and 2) a copy of the student’s candidacy proposal. After review of the student’s letter and candidacy proposal, the Steering Committee can submit additional questions to the student regarding his/her proposal. The Steering Committee will review the responses and determine if a thesis is approved; it is possible for the Steering Committee to approve the thesis without additional questions. If a thesis is not approved by the Steering Committee and the question cannot be successfully resolved, then the request can be appealed to the Executive Committee for review. The appeals can be made in writing to the committee via Heidi Deethardt, 206 Cushing Hall, [MSE-list@nd.edu](mailto:MSE-list@nd.edu).

**Qualifying Exam**
Students will follow the qualifying exams policy guidelines as set out in the home department policies.

**The Candidacy Examination**

Students will follow the candidacy examination policy guidelines as set out in the home department policies.

**The Dissertation and Defense**

In addition to the thesis approval process by the Steering Committee previously indicated, students will follow the dissertation and defense policy guidelines as set out in the home department policies.

**VI. FACILITIES AND SERVICES**

**A. Library**

The University Library system consists of a number of libraries. Circulation policies and operating hours are available at each of the libraries. Students should make themselves aware of the resources the libraries provide and become more familiar with them by visiting the University library website, [http://library.nd.edu/](http://library.nd.edu/).

**B. Computing Facilities**

The Office of Information Technologies (OIT) oversees an extensive variety of computers, workstation clusters, and personal computer facilities throughout campus. The University has a wide range of software and printing services available for use by all students. For a complete current listing of University facilities students should visit [http://oit.nd.edu](http://oit.nd.edu).

The Center for Research Computing (CRC) at University of Notre Dame is an innovative and multidisciplinary research environment that supports collaboration to facilitate multidisciplinary discoveries through advanced computation, software engineering, data analysis, and other digital research tools. The CRC is comprised of four main groups with complementary expertise: computational scientists, software development, Center for Social Science Research, and high performance computing. For more information on the CRC visit [https://crc.nd.edu/](https://crc.nd.edu/).

**C. Laboratory Facilities**

Students may work in a wide variety of laboratories across the University campus. These may be laboratories specific to the student’s research group, or shared facilities that are supported by user fees.

**D. Office Facilities**

All full-time graduate students have access to personal office space. Offices are typically shared with other students. Each student will also have a mailbox located in or near the main administrative office in the building to which the student has been assigned. Students are
expected to maintain professional office environments, to maintain a neat office, and to be respectful and courteous to their office mates and others in their office environment.

E. Copying Facilities
There are many copying facilities on campus, with services available at a charge. Many small machines are located in Hesburgh Library, branch libraries and home departments. Students should check with the administrative staff or their advisor to learn about local resources.

F. Student Government Service
Graduate students are responsible for the activities of the Graduate Student Union (GSU). Through a council of elected officers, appointed officers, and representatives from the departments of its constituent colleges, the GSU provides a variety of services and represents its membership on various University councils and committees. It publishes the bimonthly GSU newsletter, conducts a graduate orientation program, and sponsors workshops, travel grants, and various social and cultural activities. The GSU is the graduate students’ official liaison with University administration, the Office of Student Activities, and the Library Administration. The GSU finances operations through a yearly fee assessed on all graduate students. The GSU maintains offices in 219 LaFortune Student Center, 631-6963; their website is: http://www.gsu.nd.edu/.

G. Health and Counseling
There are additional services available to graduate students, described in the Bulletin of Information or on the web at: http://graduateschool.nd.edu/resources-for-current-students/.

University Health Services, located in the University Health Center, 631-7497, provides immediate, follow-up, and ongoing health care. The services provided include outpatient clinics, dispensing medication, administering allergy injections, laboratory and x-ray facilities, and a 25 bed inpatient unit. Health insurance is required of all international and full-time students. The University offers a plan for all students. A student's spouse and children have the option of purchasing health insurance through this plan. More information can be obtained by calling 631-6114. The University Counseling Center, located in the University Health Center, 631-7336, offers professional services to all graduate students and their families.

The University Counseling Center's is available to assist students in meeting the challenges that are an integral part of their Notre Dame experience. Their professional staff of licensed psychologists, social workers, psychiatric providers, and masters-level psychologists-in-training are highly skilled in helping students address the difficulties they may encounter, and empowering them to make the most of the opportunities available to them at Notre Dame. The University Counseling Center specializes in treating the mental health concerns that are prevalent in a diverse university student body. The University Counseling Center is located in the University Health Center and can be reached at 631-7336. More information can be found by visiting https://ucc.nd.edu/. All services are free of charge and confidential.
The University has excellent athletic and exercise facilities; most are available free of charge. More information can be found at https://recsports.nd.edu/.

H. Career and Placement
The University’s Graduate Career Services provides assistance with post-graduate placement and professional development through online services and the guidance of its graduate career consultants.

I. International and Religious Services
The University supports an International Student Affairs Office, 205 LaFortune, 631-5243, which aids in immigration matters, serves as liaison with sponsoring agencies and governments, and promotes interaction within the University. The International Student Organization (ISO), 204 LaFortune, is a club for interested students.

Campus Ministry, 116 Coleman-Morse Center, 631-7800, offers programs and organizations to serve students’ spiritual needs across a full range of faith traditions.

J. Graduate Student Life
A unit within the Division of Student Affairs and in cooperation with the Graduate School, Graduate Student life (http://gradlife.nd.edu/) is committed to enhancing the educational experience and quality of life for Notre Dame students pursuing advanced degrees. The Graduate Student Life website contains reference links for special events and programs, family resources and information regarding campus life in general. A helpful Q&A weblog to answer questions is also featured.
APPENDICES

A. ACADEMIC INTEGRITY

In questions involving academic integrity, the student is referred to the general policy found in the Graduate School Bulletin of Information. The department expects all students to maintain and promote the highest standards of personal honesty and professional integrity. These standards apply to examinations, assigned papers, projects and preparation of the thesis or dissertation. Violation of these standards, which includes, but is not limited to cheating in examinations, plagiarism and fraudulent practices in conducting research or reporting the results of such research, may result in suspension or dismissal.

Primary authority for judgment and decision on matters of academic integrity lies with the course instructor for issues that arise in the classroom, or the faculty research advisor for issues that arise in research. Unsettled disputes should be referred first to the director of graduate studies in the student’s home department and next to the student’s home department chair, each of whom can serve as arbiters at the department level. Any further appeal should be directed to the Graduate School.

B. FACULTY

For faculty affiliated with the Materials Science and Engineering program, click on the following:
https://nano.nd.edu/faculty/?dept=&program=materials-science&id=
D. MATERIALS SCIENCE AND ENGINEERING GRADUATE COURSES

Material Structure

CBE 60561 – Structure of Solids (Paul McGinn, Spring 2019). This class seeks to provide students with an understanding of the structure of solids, primarily as found in metals, alloys, and ceramics applied in technological applications. The structure of crystalline solids on the atomic level as well as the microstructural level will be discussed. Imperfections in the arrangements of atoms will be described, especially as regards their impact on properties. The study of structure through X-ray diffraction will be a recurring theme. A sequence of powder diffraction laboratory experiments (four to five class periods) also will be included.

CHEM 60618 – Chemical Crystallography (Allen Oliver, Spring 2018-19). This course covers the theoretical and practical aspects of Small Molecule X-ray Crystallography. There will be both lecture and laboratory sessions with this course. Topics covered include: crystal growth, the diffraction experiment, space group analysis, symmetry, structure solution and refinement, powder diffraction, use of typical software for diffraction studies. The laboratory session will cover the practical aspects of crystal selection and the use of X-ray diffractometers.

CHEM 60438 – Polymer: Principle to Practice (Haifeng Gao, Spring 2018-19). This course offers the basic physical and organic chemistry knowledge in polymerization reactions. Topics to be covered include mechanisms of polymerization reactions; polymerization kinetics and thermodynamics; relationship of physical properties to structure and composition; correlations of applications with chemical constitution; functional polymers for medicines and electronics. The course is recommended for students with special interest in polymer materials and future plan on polymer research and professional studies.

CE 60382 – Actinide Chemistry (Amy Hixon, Fall 2018-2019). This course is intended to provide students with a basic understanding of the fundamental chemical and physical properties of actinide elements. Lectures will focus on solution chemistry, bonding, kinetics, and thermodynamics in the context of the behavior of actinides in the environment and within the nuclear fuel cycle. Particular emphasis will be placed on solution chemistry of the actinides and interactions at the solid-water interface.

CBE 60457 – Polymer Science & Engineering (Ruilan Guo, Fall 2018). This course is an intermediate level introduction to the fundamental chemistry and physics of polymer materials. The course is designed to meet the needs of students in all science and engineering disciplines who are interested, or already engaging in polymer related research. The lectures will focus on the underlying concepts and principles in polymer materials, emphasizing the interrelationships between synthesis, structure, processing, properties and performance, and demonstrate them in the context of their everyday use as well as real-world advanced engineering applications. Major topics in polymer chemistry, physics and engineering will be covered including: general introduction of polymers, major classes of polymerization reactions and kinetics, microstructure and morphology, polymer properties (thermal, mechanical, etc.), polymer thermodynamics,
polymer characterization techniques, and plastics engineering and processing methods. The successful students will emerge from the course with a current, sound knowledge of polymer concepts and an ability to apply them in career situations.

**CBE 60725 - Principles of Molecular Engineering (Matthew Webber, Spring 2018-19).** The objective of this course, intended for both upper level undergraduate and graduate students, is to illustrate the emerging field of molecular engineering. By fusing concepts from chemistry and materials science, molecular engineering seeks rational design of chemical building blocks for organized systems and materials. Students will gain a fundamental perspective for how non-covalent interactions and designed molecular motifs can dictate the structure, function, and properties of resulting engineered systems. This will include an appreciation for the role on intermolecular forces in governing the behavior of these molecules as they interact with each other and with their environment (typically a solvent). Additionally, illustrative examples will point to the power of strategies rooted in principles of molecular engineering to create highly controlled and functional materials. Topics will include: non-covalent interactions, molecular design, thermodynamic driving forces, solvent effects, molecular self-assembly, supramolecular chemistry, molecular & materials characterization techniques, and applications of molecular engineering for diverse uses in energy, medicine, computing, formulation science, industrial applications, and food sciences.

**Nanostructure Materials**

**CBE 60577 – CHEM 60577 - Nanoscience and Technology (Paul Bohn & Alexander Mukasyan Fall 2018-19).** This course focuses on the unique scientific phenomena that accrue to matter with characteristic nanometer-scale dimensions and on the technologies which can be constructed from them. Special optical, electronic, magnetic, fluidic, structural and dynamic properties characteristic of nanostructures will be addressed.

**AME 60679 – Nanoparticles in Biomedicine (Ryan Roeder 2018).** Nanoparticle science and engineering will be introduced including the processing (synthesis and surface modification), structure (physical and molecular), and functional properties (biological, electrical, magnetic, mechanical, optical, X-ray, etc.) that enable biomedical applications in drug delivery, imaging, sensing, and tissue regeneration.

**Electronic Materials**

**EE 60556 – Fundamentals of Semiconductor/Physics (Suman Datta, Fall 2018-19).** Treatment of the basic principles of solids. Topics include periodic structures, lattice waves, electron states, static and dynamic properties of solids, electron-electron interaction transport, and optical properties.

**PHYS 50501 – Intro to Solid State Physics (Bruce Bunker, Fall 2018-19).** The course is intended to introduce the principles of the behavior electrons and phonons in solids, advanced concepts and applications, such as low-dimensional systems and superconductivity, and set the
conceptual framework needed for future study and graduate research in condensed matter physics or technology-related industry. Topics will include: crystal structure and diffraction, phonons and heat capacity, free electron gas and elementary band theory, semiconductors, magnetism, and superconductivity.

**CBE 60435 – CHEM 60435 - Electrochemistry and Electrochemical Engineering (Paul Bohn, Fall 2018).** This course addresses the fundamentals and applications of technologies that rely on heterogeneous electron transfer reactions. The first part of the course addresses fundamental aspects of electron transfer reactions at electrified interfaces, including band structure of metals and semiconductors, electrochemical potentials, electron transfer kinetics and Marcus theory, potential step and potential sweep experiments, hydrodynamic electrochemistry, potentiometry and ion-selective electrodes, impedance measurements, and electrochemical instrumentation. The second part of the course addresses applications to energy storage (batteries, fuel cells, supercapacitors), energy conversion (photovoltaics), bioelectrochemistry, including neurochemistry, corrosion, and electrolysis and electroplating.

**PHYS 90507 – Topology and Dirac Fermions in Condensed Matter (Badih Assaf, Fall 2018).** This course is an introduction to the burgeoning field of topological and Dirac matter. It covers the following topics: Dirac, Weyl and Majorana fermions, the Jackiw-Bell solution to the Dirac equation, the Berry phase, topological invariants, the band structure of graphene and experimental proofs of its Dirac nature, toy models of topological systems (Kane-Mele, Su-Schrieffe-Heeger, ...), realistic topological materials and their band structure, experimental observables of non-trivial topology (quantum spin Hall effect, band-inversion, ...).

**Material Surfaces and Interfaces**

**CBE 60625 – Principles of Heterogeneous Catalysis (Jason Hicks, Spring 2019).** This course will provide a comprehensive overview of heterogeneous catalysis with particular focus on catalyst synthesis, modern characterization techniques, kinetics, and reaction mechanisms for energy-related applications. Emphasis will be placed on 1) understanding the synthesis and properties of a variety of solid catalysts including carbides, phosphides, zeolites, bimetallic catalysts, tethered catalysts, and metal-organic frameworks, and 2) in-situ/operando techniques to aid in the design of new materials.

**CE 60300 – Geochemistry (Jeremy Fein, Fall 2018).** An introduction to the use of chemical thermodynamics and chemical kinetics in modeling geochemical processes. Special emphasis is placed on water-rock interactions of environmental interest.

**CE 606355 - High-Temperature Geochemistry (Clive Neal, Spring 2019)** This course examines the generation and evolution of magma from a physicochemical standpoint. Using actual geochemical datasets and samples in conjunction with research papers will allow the student to develop the skills for formulating petrogenetic models that are thermodynamically
viable. These skills will be used in their individual research projects. The student is evaluated by two exams, weekly homework assignments, and a research paper.

**EE 60568 – Fundamentals of Photonics (Scott Howard, Spring 2018).** The fundamental physics and engineering of photonic devices will be explored in this class. We will start with Maxwell's equations and study light propagation and interaction with materials, diffraction theory, photon statistics, waveguides, lasers, and optoelectronics. Experience with vector calculus, frequency domain (Fourier) analysis, and previous coursework in electromagnetism are strongly recommended. Appropriate for both graduate students and advanced undergraduate students.

**Biomaterials**

**AME 50571 – Structural Aspects of Biomaterials (Donny Hanjaya-Putra, Fall 2018-19).** Structure and mechanical functions of load bearing tissues and their replacements. Natural and synthetic load-bearing biomaterials for clinical applications are reviewed. Biocompatibility and host response to structural implants are examined. Quantitative treatment of biomechanical issues related to design of biomaterial replacements for structural function. Material selection for reconstructive surgery is addressed. Directions in tissue engineering are presented.

**AME 60672 – Cell Mechanics (Glen Niebur, Fall 2018).** The effects of mechanical loading on cells are examined. Mechanical properties and material structure of cell materials are reviewed. Filaments, filament networks and membranes are examined. Mechanics of flow induced effects, adhesion cell-substrate interactions, and signal transduction are examined. Experimental techniques are reviewed.

**CBE 60888 – Cellular and Physical Principles of Bioengineering (Basar Bilgicer, Spring 2018-19).** This course covers the breakdown of biological systems at molecular, cellular and tissue levels. It evolves to the design and synthesis of biomaterials at a molecular scale used in manipulating and targeting biological systems, including biotechnology and biomedical engineering. For these purposes, we will learn what is inside a cell, molecular machines, nerve impulses, binding thermodynamics and kinetics in biological systems, chemical forces and molecular self-assembly.

**Materials Characterization**

**CHEM 60532 – Optical Spectroscopy (Ken Kuno / Greg Hartland, Fall 2017).** Principles and applications of spectroscopic measurements and instrumentation. Atomic and molecular absorption, emission, fluorescence, and scattering, emphasizing physical interpretation of experimental data.

**CBE 60727 – CHEM 60727 – Ambient methods for Surface Characterization (Merlin Bruening, Spring 2019).** This course develops fundamental principles for characterizing surfaces and interfaces, particularly thin films, using infrared spectroscopy, ellipsometry,
electrochemistry, and contact angle measurements. The material will cover reflection of light from surfaces, which is relevant to surface infrared spectroscopy, surface plasmon resonance and ellipsometry, surface energies, adsorption isotherms, and some fundamental aspects of electrical double layers, zeta potentials, and mass transport in electrochemistry.

CBE 80603, EE 80603 – Transmission Electron Microscopy (Sergei Rouvimov, Fall 2017)
Course is an introduction to the fundamental basis and operations of transmission electron microscope and is required for all students who plan using the TEM in their research. Goals: The course goal is for the students to become competent, research-level experts in transmission electron microscopy. They will understand the functions of the TEM and how it works. They will be competent in basic operating techniques, and ready to learn more advanced ones as needed There will be a lectures (2 per week) and laboratory demonstration (3 hours/week). Topics will include: Electro-optics of the TEM - Image formation and imaging modes - Diffraction theory and Diffraction patterns - Dark and bright field imaging - Image interpretation - High resolution microscopy and Lattice imaging - Sample preparation.

Phase Equilibria

PHYS 60050 – Computational Physics (Zoltan Toroczkai - Ferenc Molnar, Spring 2018-19).
This course will provide a basic foundation in the skills and knowledge needed for computational physics. The course has three major parts: (1) Programming basics, with Python; (2) algorithms and methods, frequently used in computational physics and (3) physics projects for turning numerical calculations into solutions to real problems. Topics will include foundations of programming, principles of numerical analysis, interpolation and extrapolation, methods for solving ordinary and partial differential equations, random processes, Markov Chains, basic statistics, graphical representations. Applications include problems from classical physics (mechanics, electrodynamics), statistical mechanics, nuclear physics, basic network science and machine learning. The main goal of this course is to introduce the students to computational thinking in solving physics problems. In that sense this is not a numerical analysis math course but a course about how to tackle a physics problem with a computer, how to perform computational "experiments" to answer questions about a physical system.

CBE 60547 – Modern Methods in Computational Molecular Thermodynamics and Kinetics (Bill Schneider, Fall 2019).
This course will introduce the basis of modern approaches to computing the thermodynamics and kinetics of gas-phase, condensed-phase, and surface chemical reactions from first principles. Quantum chemical wavefunction and density functional approaches for treating the electronic structure of molecules, solids, and surfaces will be described. Optimization methods and statistical mechanical techniques for determining structures, spectroscopies, and thermodynamic and kinetic properties will be covered. Software for calculating these properties will be introduced and applied in hands-on exercises and a class project.

CBE 60553 – Advanced Chemical Engineering Thermodynamics (William Schneider, Fall 2017).
This course is focused on an advanced treatment of thermodynamic concepts. An
introduction to molecular thermodynamics is given, followed by detailed treatments of phase equilibrium, equation-of-state development and activity coefficient models.

**CBE 60642 – Molecular Thermodynamics (Jonathan Whitmer, Fall 2019).** This course examines advanced topics in thermodynamics and statistical mechanics, including phase transitions, lattice models, renormalization group theory, critical phenomena, physical meaning and interpretation of correlation functions, classical partition functions and collective variables, liquid theory, molecular simulations of fluids and ordered phases, structure and dynamics of complex media, and supercooled and glassy materials.

**Modeling**

**AME 60649 – Molecular Level Modeling for Engineering Applications (Tengfei Luo, Fall 2017).** This graduate level course is intended for engineering graduate students with interests in the simulation of materials and studying their properties at the molecular level using different atomistic simulations techniques. This course will introduce basics of statistical thermodynamics and classical Monte Carlo and molecular dynamics simulations. With the fundamentals, students will learn how to use the knowledge and techniques to study engineering problems such as mass diffusion and heat transfer. It will also emphasize hands-on exercises in which student will use these techniques to model different materials including gas, liquid, solid, the phase transition among these different phases. Structural, flow and thermal properties of materials will also be studied. Students will be required to program their own code for small projects and will be using open source software, such as LAMMPS, for larger projects.

**Quantum Mechanics**

**CHEM 60648 – Quantum Mechanics II (Steven Corcelli, Spring 2018).** Advanced topics in quantum chemistry; electron spin and the Pauli principle; methods for obtaining quantum mechanical electronic structure: semiempirical methods, Hartree-Fock self-consistent-field method, many-electron perturbation theory, configuration interaction, coupled cluster methods, and density functional theory; time-dependent density functional theory; nonadiabatic quantum dynamics; mixed quantum mechanics / molecular mechanics methods.

**CHEM 60649 – Quantum Mechanics (Arnaldo Serrano, Fall 2018-19).** A survey of quantum mechanics at an intermediate level, oriented toward problems of chemical interest. Relevant mathematical concepts are developed, including Dirac notation, matrix algebra, orthogonal functions, and commutator relations. Topics covered include harmonic oscillators, central field problems, wave packets, angular momentum, and approximation methods.

**EE 60587 – Quantum Mechanics for EE (Craig Lent, Fall).** The course focuses on those aspects of quantum theory that are of particular relevance to electrical engineering. It is intended to give seniors and first-year graduate students a working knowledge of quantum mechanics at a level sufficient to illuminate the operation of standard and advanced quantum devices. Topics include classical mechanics versus quantum mechanics, early quantum theory,
Schrödinger formulation, time-dependent and time-independent Schrödinger equation, Dirac formulation, Bloch theorem, magnetic effects, open quantum systems, and density matrices.

**PHYS 70007 – Quantum Mechanics I (Morten Eskildsen, Fall 2019).** General Hilbert Space formulation of Quantum Mechanics; Schrödinger vs. Heisenberg picture; harmonic oscillator; the Coulomb problem; the Bohm-Aharonov effect; the theory of angular momentum; EPR correlations and Bell's inequality.

**PHYS 70008 – Quantum Mechanics II (Carol Tanner, Luca Boccioli, Spring 2019).** Continuation of Quantum Mechanics I. Symmetries and conservation laws; Bose-Einstein and Fermi-Dirac statistics; elementary approximation methods; scattering theory realistic hydrogen atom; advanced approximation methods; partial wave expansions; the optical theorem; introduction of the Feynman rules; relativistic quantum mechanics and the Klein-Gordon theorem.

**AME 60632 – Physical Gas Dynamics (Eric Jumper, Fall 2018).** An introduction to quantum mechanics, internal structure, and quantum energy states of monatomic and diatomic gases. Application to chemical reactions, dissociating gases, and ionized gases. High temperature properties of air.