Northwestern | McCORMICK SCHOOL OF ENGINEERING

GRADUATE PROGRAM

Roadmap for the PhD | New Student Orientation

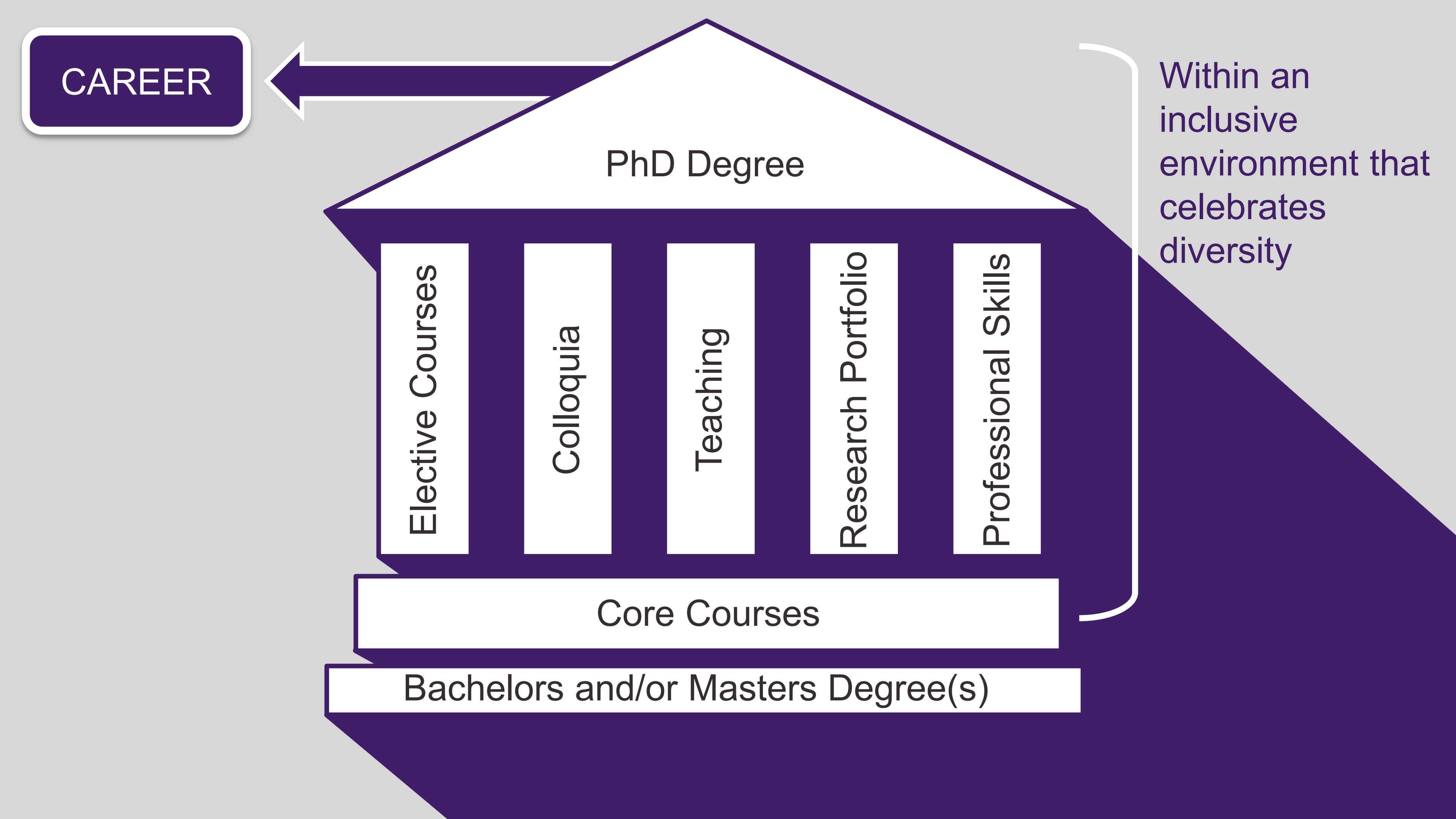
Materials Science and Engineering

Prof. Ken Shull | Director of Graduate Studies
Prof. Jon Emery | Assistant Director of Graduate Studies
Prof. James Rondinelli

NOTE: ALL SLIDES AVAILABLE ON CANVAS

Program Educational Outcomes

- Demonstrate advanced proficiency in the science and engineering of materials.
- Demonstrate the ability to identify and solve unique and important scientific/engineering problems through research that applies experimentation, theory, modeling, and/or simulation.
- Manage research projects and function on multidisciplinary teams.
- Communicate effectively with both technical and non-technical audiences, including networking and self-promotion.
- Show awareness of professional and ethical responsibilities, safety in experimental research, and non-scientific career goals.


CAREER
PhD Degree
Elective Courses
Colloquia
Teaching
Research Portfolio
Professional Skills
Core Courses
Bachelors and/or Masters Degree(s)
Within an inclusive environment that celebrates diversity

Science of Materials

Fundamental Foundations

- Physical Laws, Formalisms, Concepts

Symmetry (Breaking)
Group Theory
Electrodynamics
Quantum Mechanics
Statistical Mechanics
Thermodynamics
Classical Mechanics

Materials Science Foundations

- Analyses of Phases in the Presence of Fields

Model Formulation
Equilibrium States
Electronic Structure: Bonds & Bands
Kinetics: Phase Transitions & Transport
Order Parameters, Symmetry Breaking
Excitations
Physical Atomic Structure, defect(free)
Microstructure

Engineering Foundations

- Structure/Property & Processing Property Relationships

Constitutive Relationships
MEMOTP Properties
Transformations
Interface Properties

Coursework | Years 1 and 2

- Usually enroll in 3 courses per quarter in Year 1
- 6 Core Courses (all in Year 1)
- 6 Elective Courses
  - At least 2 MSE 400-level courses
  - Have an M.S.? Credit for up to 3 courses, with the option of up to two 499 (indendent study) courses counting towards the requirement

Core Curriculum Roadmap

- The roadmap is both a guide to the course terrain and a compass to navigate the intersections among courses
  - The core course route is selected by the faculty, but they won’t choose your ultimate route, which includes specialization through electives (consult PI)

- Only you know what destination you want to reach
  - The roadmap will help you identify some of the key landmarks and points of interest you will want to visit

Fundamental Foundations
Materials Science Foundations
Engineering Foundations

SUMMER	FALL	WINTER	SPRING	SUMMER

Preparation, PSP

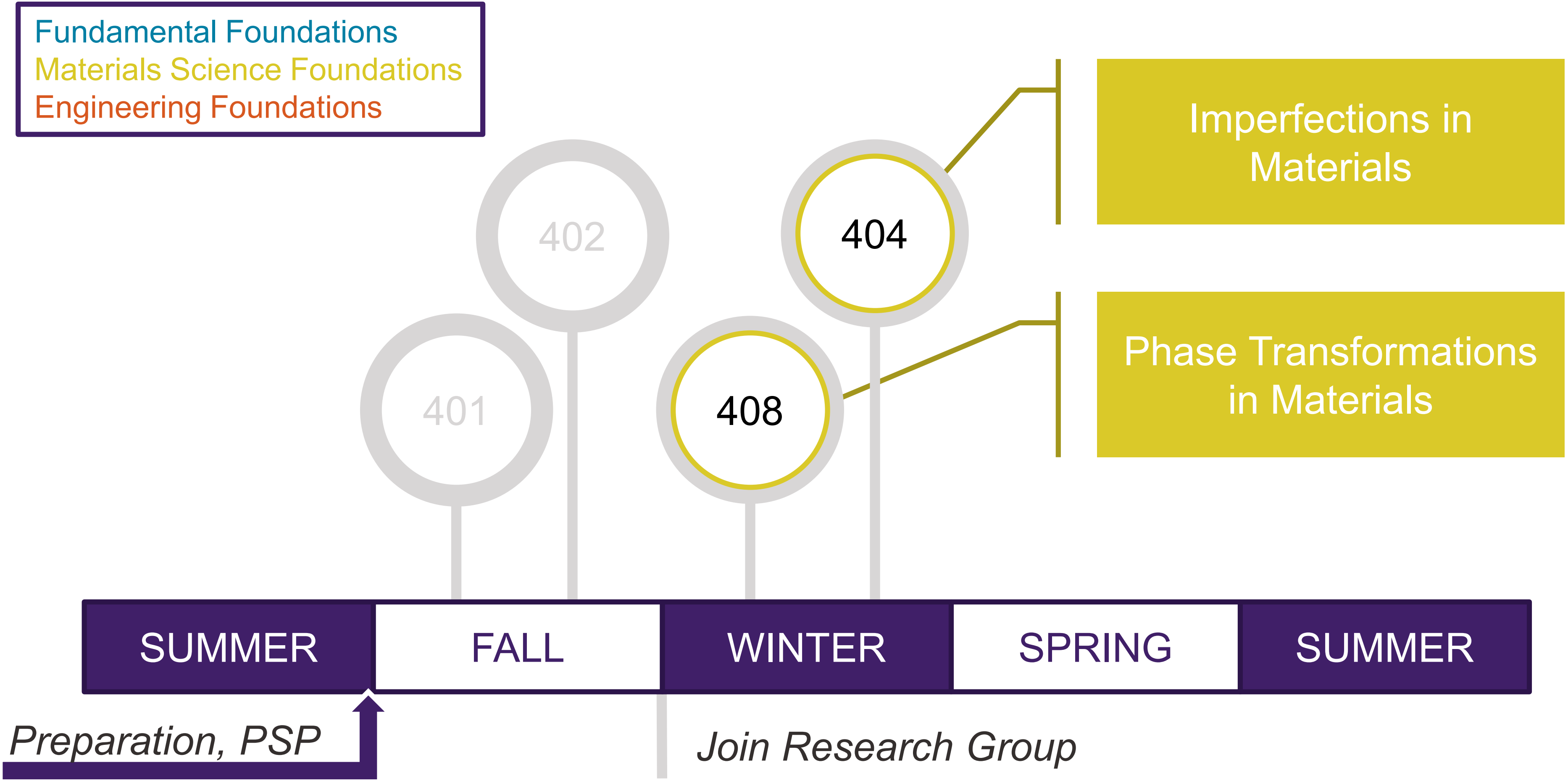
Fundamental Foundations
Materials Science Foundations
Engineering Foundations

402 — Structure of Materials

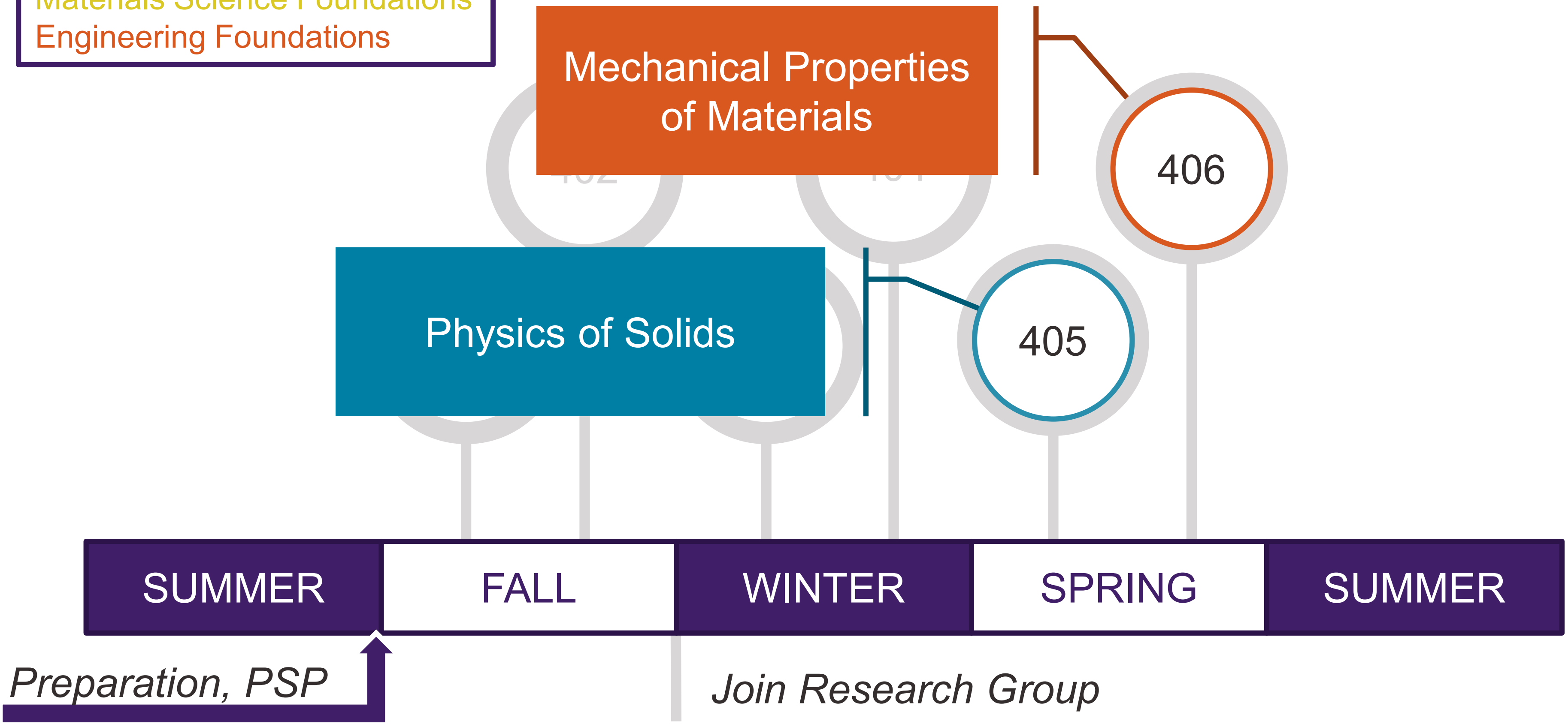
401 — Chemical and Statistical Thermodynamics

SUMMER	FALL	WINTER	SPRING	SUMMER

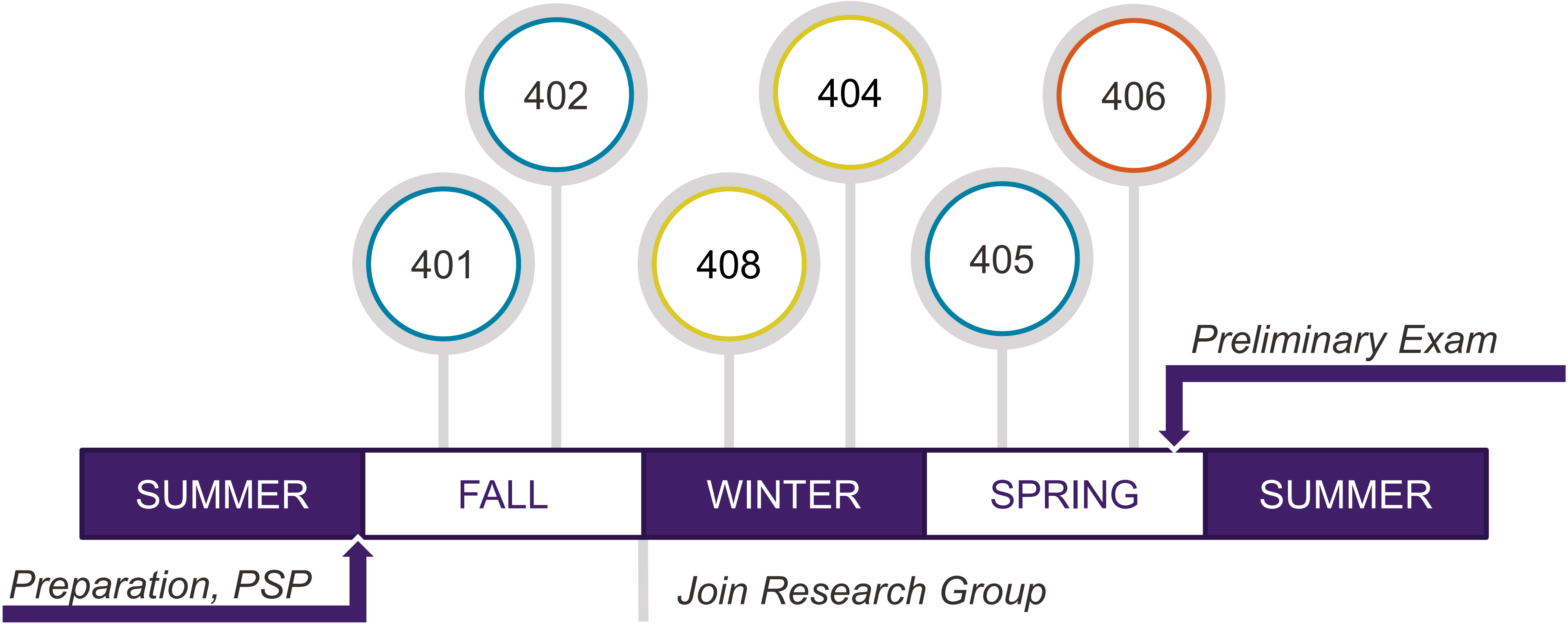
Preparation, PSP


Fundamental Foundations
Materials Science Foundations
Engineering Foundations
402
404
Imperfections in Materials
401
408
Phase Transformations in Materials
SUMMER
FALL
WINTER
SPRING
SUMMER
Preparation, PSP
Join Research Group

Fundamental Foundations
Materials Science Foundations
Engineering Foundations

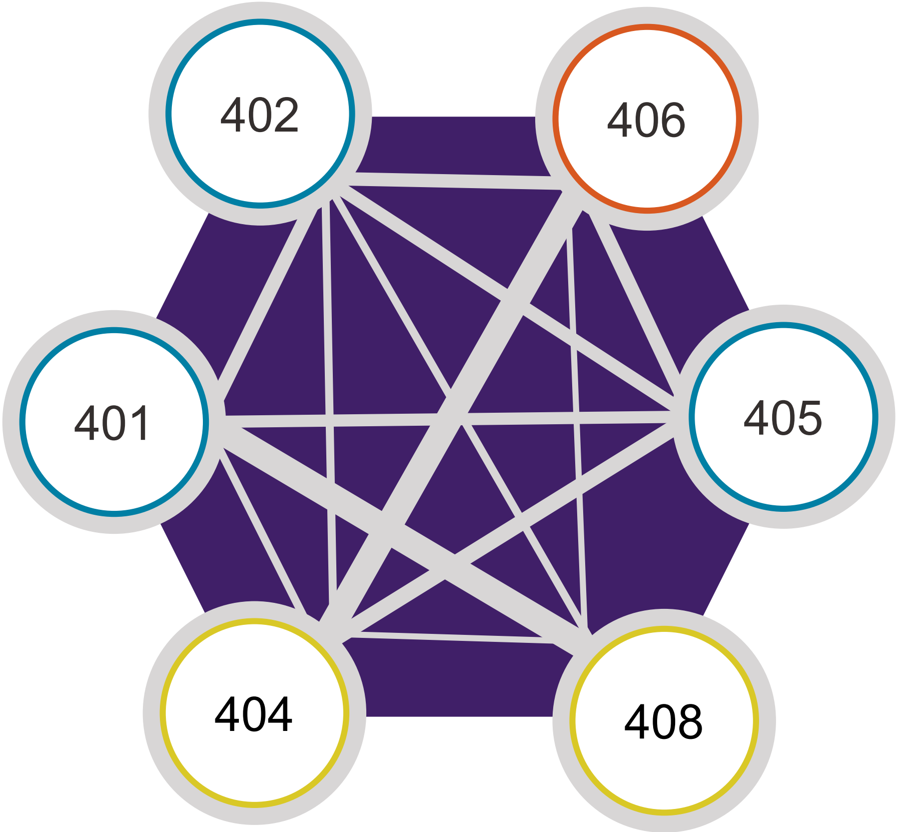


Fundamental Foundations
Materials Science Foundations
Engineering Foundations



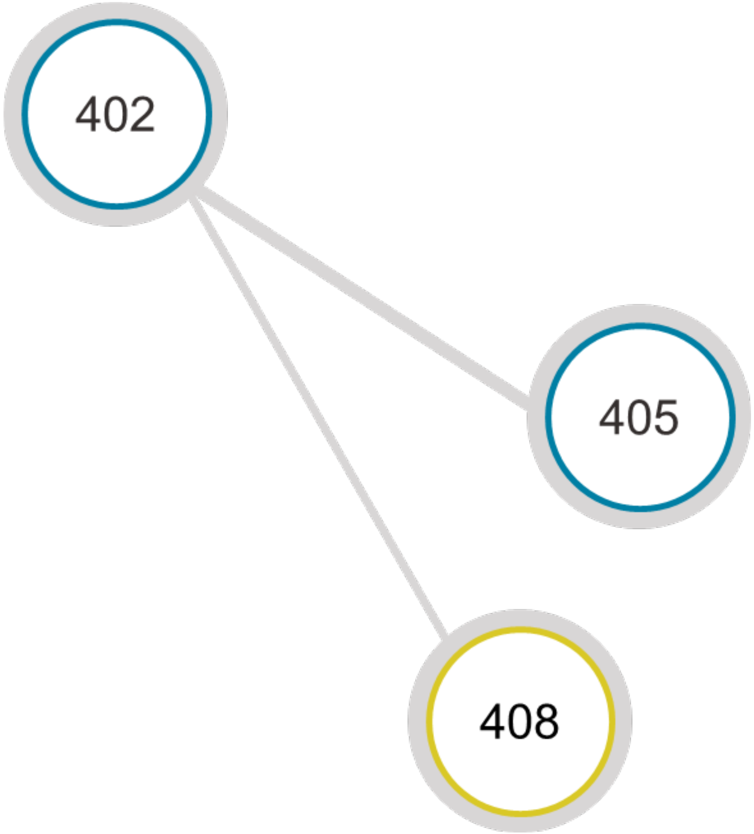
Interactions

401Thermodynamics
402 Structure of Materials
404 Imperfections in Materials
405 Physics of Solids
406 Mechanical Properties of Materials
408 Phase Transformations in Materials



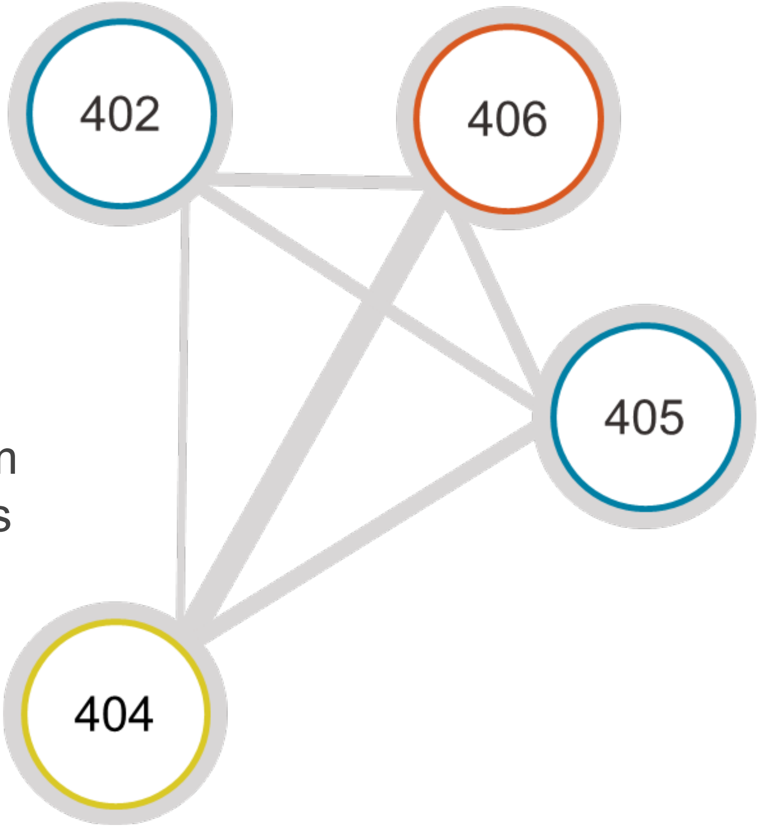
Interactions | Example 1

- Students learn in 402 how to describe symmetry breaking that accompanies phase transitions.
- These transitions are formulated mathematically in 408, and lead to different physical properties, e.g., electrical conductivity described in 405 and shown to depend on changes in band structure and bonding.



Interactions | Example 2

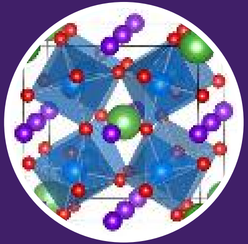
- Students learn in 402 the constitutive relationships for linear elasticity and restrictions imposed crystal symmetry.
- The microscopic origin of mechanical properties are described in 406 and arise from changes in bonding (405). Quantitative values for different materials are discussed in connection with the implications on strengthening due to dislocation motion.
- The formation and interaction among dislocations in imperfect materials are described in 404.



2020-2021 Core Course Instructors

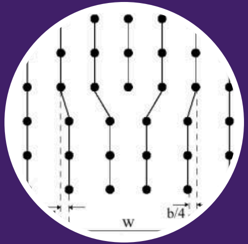
401

- Lauhon
- Luijten



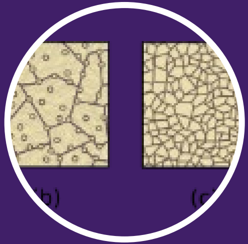
402

- Rondinelli
- Shull



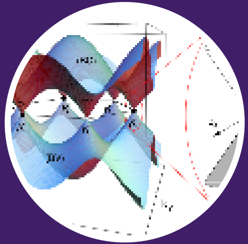
404

- Haile
- Seidman



408

- Voorhees



405

- Hersam

406

- Dunand
- Emery

Fall 2020 Class Format and Expectations

Format

- Hybrid mode (in-person and/or virtual)
- Recorded lectures
- Various assessments (quizzes, homework, orals)

Recommendations

- Form virtual study groups
- Seek help during office hours
- Make accommodation requests early with AccessibleNU

Expectations

- Practice COVID-19 policies
- Zoom etiquette
- Attend and participate (come with questions) in class (virtually) and as frequently as possible
- Read assigned content prior to lecture
- Review recorded lectures

Pre-course Assessments (due 9/10)

- Why?
  - MSE student background is diverse.
  - Want to:
    - Provide students with a pre-course assessment of preparedness.
    - Provide students with an impetus for self-guided study.
    - Provide students with resources for study.
- **These are intended to advise and guide, not judge.**
- Don't worry - only the aDSG (Emery) sees the results with names attached.
- After completion → view study recommendations and construct study plan.
- Note – a "low" score on a pre-course assessment doesn't mean anything!

Fall Term Academic Tutorials/Support

- Additional resources:
  - Pre-course assessment solutions
  - Optional (but *highly encouraged*) first-week background readings/discussion on 401 content using *Perusall.*[*]
  - *Perusall* comment-inspired discussion sections during week of Sept. 21st.
  - Background lectures (phase diagrams, VESTA) week of Sept. 21st.
  - Mathematics toolbox tutorials starting week of Sept. 28th.
    - Linear algebra
    - Calculus
    - Fourier Series
    - Complex variable

[*]Kasap and Porter and Easterling

CORE COURSE OUTCOMES

Your Success in the Core Curriculum

- The curriculum is organized to include targets that can be accurately assessed after a course is completed
- The desired outcomes for each core course are itemized on the following slides
- The outcomes are written to describe skills you should be able to perform
- The outcomes were identified from an inclusive (faculty and staff) review process

401 Course Outcomes

- Apply the three laws of thermodynamics to various systems and explain the implications of the three laws.
- Determine equilibrium conditions of systems by calculating multiplicities and free energies and explain the minimization of free energy as a driving force for phase transitions and entropy as the maximization of multiplicity.
- Derive thermodynamic properties using the combined statement of the first and second law utilizing Maxwell relations, derivation of the partition function, and extraction from phase diagrams.
- Utilize the partition function to solve for thermodynamic properties in a variety of model systems and explain the partition function as the connection between microscopic and phenomenological behavior in materials.
- Construct eutectic and miscibility gap binary phase diagrams from free-energy functions or curves and extract thermodynamic information from binary & ternary phase diagrams including eutectic & critical points, equilibrium compositions and amounts, and spinodal decomposition regions.
- Utilize statistical-mechanical models for mixtures, including the lattice model for binary mixtures and the regular solution model.
- Derive the Clausius–Clapeyron equation, the Gibbs-Duhem relation, and other basic thermodynamic identities; explain these relationships not only mathematically, but also conceptually, as well as their implications.
- Apply mean-field approximations for phase transitions and understand phase transitions phenomenologically in terms of Landau theory.
- Calculate vapor pressures and equilibrium adsorption concentrations from microscopic models and describe surface phenomena including the Langmuir isotherm.
- Apply the Nernst, Nernst-Planck and Poisson-Boltzmann equations and explain the concepts of electrochemical potential and screening.

402 Course Outcomes

- Identify point and translational symmetry elements in 2D and 3D crystals
- Deduce the number and equivalency of tensor coefficients for different physical properties given only the symmetry of a crystalline material
- Utilize tensor operations to assess anisotropic properties of materials
- Describe how complex crystalline structures are generated from simple structures through the process of atom addition, removal, or distortion
- Construct models of physical behaviors using a symmetry-based description of structure-property relationships
- Explain how a symmetry break (transition) affects the atomic structure, exhibited symmetries, and thereby allowed properties and anisotropies
- Compare and contrast how complex noncrystalline structures are arranged in ceramics and polymers using appropriate nomenclature and explain implications on properties

404 Course Outcomes

- Apply fundamental thermodynamic principle to point defects, and compare the equilibrium defect concentration under different external situations.
- Understand different defect formation reactions in ionic crystals, and derive concentration of defects by applying the method in non-ionic systems.
- Compare different diffusion mechanisms, and calculate diffusion coefficients for different cases.
- Understand the importance of dislocations in deformation of materials, distinguish different dislocations, and apply Frank’s law to derive dislocation characteristics.
- Apply Peach-Koehler equation to calculate the interaction between dislocations, and to evaluate the dislocation motion, climbing and/or gliding.
- Understand partial dislocations via Thompson tetrahedron.
- Understand CSL theory, and can apply to simple systems.
- Apply Read-Shockley model for energy of low angle grain boundary.

408 Course Outcomes

- Describe the difference in the thermodynamics of interfaces and how they are different from that of the bulk
- Determine the stability of phases at a given temperature and composition and describe the necessary requirements for any phase change to occur
- Derive equations of generalized chemical potentials for a given total free energy and the effects that gradients in composition affect the chemical potential
- Explain the evolution of composition and size that occurs in precipitates during a phase transformation and the driving force that causes such changes
- Determine the evolution of composition as a function of time in a given diffusion scenario by solving the diffusion equation
- Solve and describe the utility of similarity solutions with regards to particle growth and how the solutions dictate the evolution of particles
- Identify the assumptions in different nucleation theories (i.e. Homogenous, heterogeneous, JMAK…) and determine the applicability of them under different scenarios
- Model the evolution of microstructure morphology using the Cahn-Hilliard equation and explain how manipulation of the overall composition, thermal fluctuations, time-step, and mesh size affects the numerical evolution

405 Course Outcomes

- Describe and apply the assumptions, implications, and limitations of the free electron theory of solids including density of states and Sommerfeld derivations.
- Apply the quantum theory of harmonic crystals to derive the dispersion relationships and thermal properties of acoustic and optical phonons.
- Identify and compare the assumptions, implications, and limitations of elementary band structure models including Kronig-Penney, tight-binding, pseudopotential, and Hartee-Fock methods.
- Calculate charge and energy transport in solids using the semiclassical model, relaxation time approximation, and Boltzmann transport equation.
- Derive the electronic properties of intrinsic and extrinsic semiconductors, including spatially varying doping profiles, using Boltzmann statistics, charge neutrality, law of mass action, continuity equation, and drift-diffusion equations.
- Describe the manifestation of interband transitions for the optical properties (absorption/emission spectra) of semiconductors including the Shockley-Hall-Read theory of recombination/generation.
- Use electromagnetic theory to derive the optical properties of metals including dielectric function, dispersion relation for transverse electromagnetic waves, and plasmons.
- Use Clausius Mossotti relation, atomic and displacement polarizability, and ferroelectricity to derive and describe the dielectric and optical properties of ionic solids.
- Derive and apply elementary models of magnetism and magnetic ordering in solids including Larmor diamagnetism, Curie's law, and Pauli paramagnetism to determine magnetization and magnetic susceptibility.

406 Course Outcomes | Lecture

- Understand all aspects of mechanical properties of a variety of materials: metals, polymers, ceramics, composites, and foams
- Explain elastic, plastic, and fracture deformation
- Determine the role of imperfections, microstructure, state of stress, temperatures, strain-rate, and environment on mechanical behavior
- Fundamentally understand the structure/property relationship for materials

406 Course Outcomes | Laboratory

- Formulate and solve simple, linear, differential equations derived from governing equations and boundary conditions to derive field values in physical systems (e.g., linear elasticity)
- Construct, using the weak formulation for linear elastic response, an FEM script using MATLAB/Mathematica/Python to solve for displacements and stresses
- Develop and assess FEM models using commercial software (COMSOL) to solve for structural deformation of materials under static load
- Evaluate some limitations of computational approaches in the mechanics of materials
- Form a basis for future application of FEM in engineering and materials science applications.

ASSESSMENT

Coursework and Research Evaluations

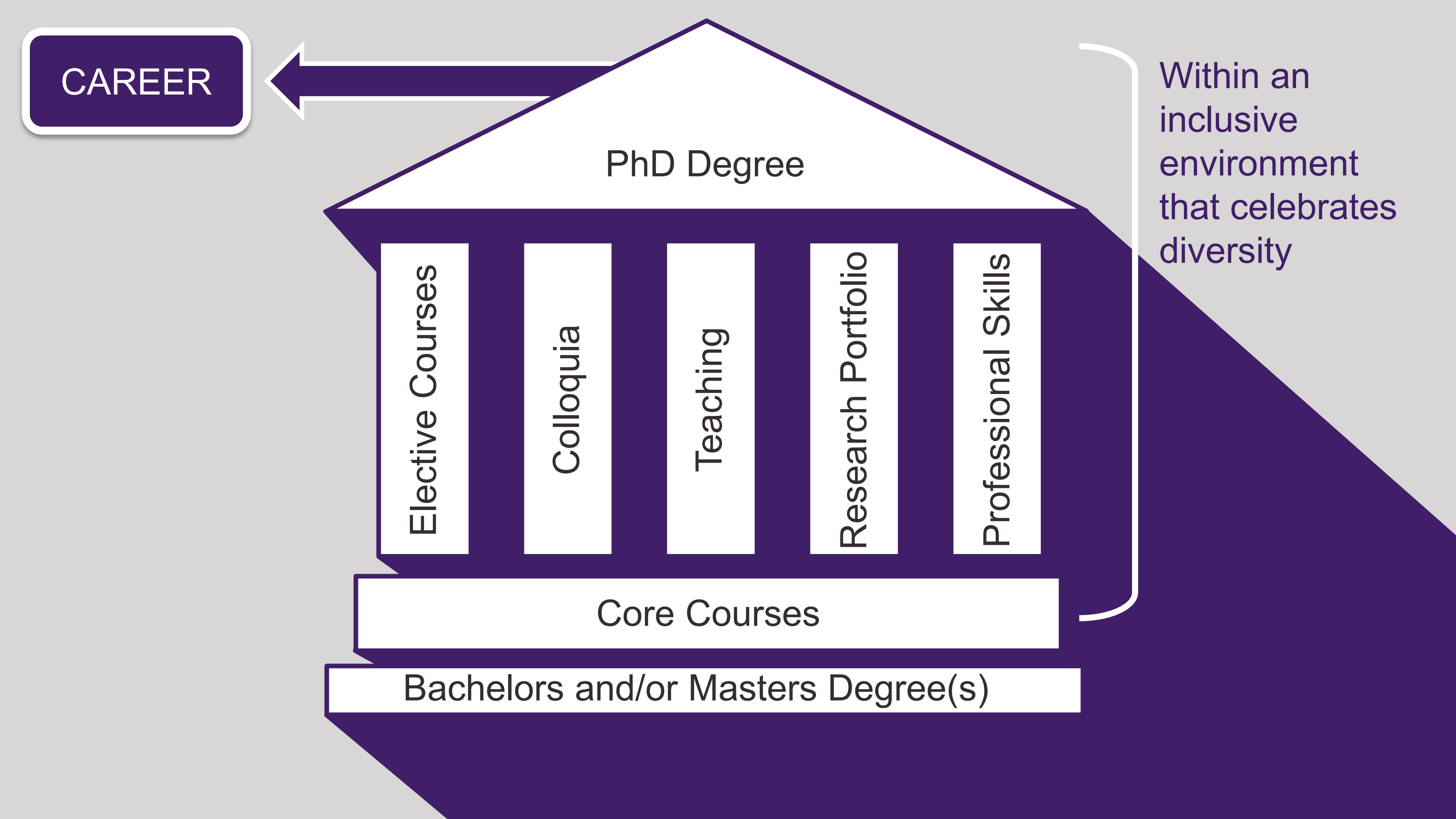
- Preliminary Exam (June of Year 1)
  - Core Course GPA > 3.2
  - Research performance assessed by adviser and faculty

- Qualifying Exam (Fall Y3, Y2 for students with MS)
  - Thesis proposal defense (admission to candidacy)
  - Evaluation of core knowledge and its application
  - Evaluation of research promise based on first two years of research

Research Evaluations

- Annual check-in following qualifier
  - Is student making reasonable progress towards the PhD degree?

- Thesis Defense
  - Significant advance in an area of MSE
    - How has the field been changed?
    - What new opportunities have been defined?
  - Typically a few first author publications


CAREER
PhD Degree
Elective Courses
Colloquia
Teaching
Research Portfolio
Professional Skills
Core Courses
Bachelors and/or Masters Degree(s)
Within an inclusive environment that celebrates diversity

Teaching | TA Requirement

- Essential part of doctoral training
- 1-3 courses (depends on time commitment)
- Commitment level varies, as does the nature of the work
- Mandatory TA training sessions

Responsible Conduct in Research: Training and Resources

- Safety first (Tuesday, in research groups)
- Ethical conduct in research and coursework
  - CITI Training: Due by December 1st
  - Gen Eng 519

- **Register for Gen Eng 519 within first year**

Managing Conflict

- Conflicts of interest are impossible to avoid completely
- Not all conflicts are “bad”
- Learning to manage conflict is part of your professional development

What should you do if you are not comfortable with an incident or situation?

Student Support and Conflict Management

- Do not wait to raise concerns
- Make use of University counseling resources
- Alice Camacho and Kathleen Stair serve as non-faculty and non-tenure line points of contact, respectively (confidential).
  - Is my concern concerning?
  - What is the best path to resolution?
- The Chair (Luijten), Director of Graduate Studies (Shull) or Assistant DGS (Emery) can be contacted at any time.

https://www.tgs.northwestern.edu/campus-life/dealing-with-conflict.html

Mental Health and Well-Being

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You should let your friends and advisor know when...

- You have not “felt like yourself” for some time
- You are having difficulty focusing on work or making progress
- Your feelings about coursework and/or research are mostly negative

ADVICE FROM CURRENT STUDENTS

In a few sentences, provide some advice for first years that you think would help them succeed in the graduate core (1/5).

- "**Don't underestimate the power of having study groups and homework buddies**. Everyone coming into the program will have different strengths and weaknesses. Working with classmates on homework can help encourage understanding of the material."
- "**Do homework as early as you can so that you can talk to the TAs** and other students about the concepts rather than just trying to finish it in time."
- "**Pay attention in class and go to class!** Ask questions, leverage off the TAs' knowledge, and use outside resources instead of the assigned textbook!"
- "The core is best viewed as a way to become familiar with the very different types of research done in the department. Thus, it is not critical to master the content of each course, but to become conversant about that area of science. Additionally, **building disparate skill sets across different course** (e.g. MATLAB/Mathematica coding, COMSOL modeling, LaTeX and Python script writing, and Vesta crystal structure visualizing) **have benefits later on**."

In a few sentences, provide some advice for first years that you think would help them succeed in the graduate core (2/5).

- “**Going to office hours and working with class mates is the best way to get through**.”
- “**Do not be afraid to ask for help and take advantage of office hours**.”
- “I found it helpful to continually review/study the material throughout the quarter even when I didn't have an exam. It made studying much better later. **Have a good sense of humor and remember to take care of yourself**.”
- “**Go to bed**.”
- “**Do not give up!**”
- “**Learn concepts not facts, and be able to apply concepts [with] math**.”

In a few sentences, provide some advice for first years that you think would help them succeed in the graduate core (3/5).

- **Take care of yourself first** and don't take the coursework too seriously. Though you should put an effort, the coursework is not the purpose of the PhD program"
- "I guess just understand that for the most part, **even though the tests and homeworks are hard, they're hard for everyone**. Just try to stay near the average, and you'll be more than fine. You do not need 4.0's, and your mental health and wellbeing is more important."
- "Work together. Everyone is coming from different backgrounds and has different strengths. **I learned the most from working with my peers who came from different backgrounds**."
- "Try on the courses you care about. Tolerate the courses you hate and just pass them. Really put effort into any computational assignments given, those you learn the most from. Math is also just an instrument for scientific thought, so **don't get too caught up in the details of the work you do, get the big picture instead**."

In a few sentences, provide some advice for first years that you think would help them succeed in the graduate core (4/5).

- Make sure to actually pay attention in class. Taking good notes helps with studying for the exam and doing homework. Problem sets are usually helpful for preparing for the exams. Make sure you understand important concepts represented in those. **Try not to fall behind in them and get them done the night before - it will literally be a nightmare**. But wait for office hours to ask the TAs rather than beating yourself up on a problem for hours if you can't figure things out. Work in groups and bounce ideas off of each other. These problem sets are not meant to be done by yourself. **Don't feel stupid if you get stuck!!!** These courses do NOT measure your worth or intelligence. You just gotta go through them as a requirement for the graduate studies. Just because you don't do well in them doesn't mean you're worthless. You are WORTHY. The coursework also does not reflect your strength in research. **Don't get hung up on the scores**. Everyone struggles at some point in these courses, and you're not alone even if it may not look like it! **Take some time to do self-care**. Know your limits. Do some meditation and take time for yourself whenever possible. Otherwise you're gonna get sick from the stress and exhaustion that come with pushing yourself too hard. It's not a sprint but a marathon. Health is the most important part of your life.

In a few sentences, provide some advice for first years that you think would help them succeed in the graduate core (5/5).

- Don't be afraid to ask for help, go to office hours and talk to your TAs. Don't worry too much about homework assignments-- **It's way more rewarding to spend time understanding concepts and studying for exams**.
- **Don't be afraid to ask questions, or admit to needing help or not knowing things. You're here to learn, not prove how smart you are.** Keep a timeline with major due dates, classes, and exams, or study and work with other people (preferably both). **The core is diverse enough that you're going to hit something that challenges you greatly, so seek help**. You'll also have chances to be the person who helps someone else in that position.
- **Surprisingly enough, people with a materials degree aren't as better of as you'd think** (assuming you don't have a materials degree), so don't let that discourage you.
- **Basically everyone will have a hard time or find material difficult, though it may not seem that way on the outside**.
- **Don't compare yourself to others**, especially regarding HW scores / test grades.
- **It's really quite hard to fail out of the program**, so spend your time and energy worrying about learning what you can instead of focusing on superficial grades.

ADVISOR SELECTION

To Do List

- CITI on-line course
- Register for Gen Eng 519
- Office of Fellowships/TGS Info
  - http://www.tgs.northwestern.edu/funding/fellowships-and-grants/index.html
- NSF GRFP deadline for US Citizens

Questions?
Coursework | Research | Practical

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