MSE 8803-A: Quantum Mechanics for Materials Science and Engineering
Spring, 2024

INSTRUCTOR: Prof. Eric Vogel, eric.vogel@mse.gatech.edu, Marcus Nanotechnology Building, Rm. 2133

CLASSES: MW, 12:30 PM – 1:45 PM, J. Erskine Love Manufacturing Building, Rm. 299

OFFICE HOURS: TBD

GOALS:
Students that complete this course will learn the fundamental underpinnings necessary to link material composition and structure with the density of states which determines the electronic, optical and thermal properties, and characterization, of almost any material class (e.g. organic molecules, semiconductors, metals, insulators).

OBJECTIVES:
The density and properties of electron and phonon states determines many of the electronic, optical and thermal properties of materials. This course provides the fundamental, quantum-mechanical underpinnings necessary to describe these states within atoms, molecules and solids. Students that complete this course will learn the fundamental underpinnings necessary to link material composition and structure with the density of states which determines the electronic, optical and thermal properties, and characterization, of almost any material class (e.g. organic molecules, semiconductors, metals, insulators). For example, Raman characterization requires understanding of allowed vibrational modes of atoms and molecules; photoluminescence requires understanding of allowed energy states and selection rules; thermal conductivity requires understanding of the phonon density of states; electron transport in solids requires understanding of band structure. A working knowledge of quantum mechanics is, therefore, necessary for a materials scientist or engineer to truly understand these properties and characterization techniques. While examples of applying this understanding to properties and characterization of specific materials will be provided as context, it should be emphasized that this class is not a properties class and will not provide broad coverage of electronic, optical and thermal properties themselves. Mathematical calculations will be required in this class; however, this course will attempt to minimize the complexity of the math to permit materials scientists and engineers to gain the necessary conceptual understanding.

REFERENCE MATERIALS: The Eisberg & Resnick book has a lot of the material that will be covered. However, to master this material, it is helpful to have several books and reference materials coming from different perspectives. The following cover aspects of the course but also cover topics that are not in this course.

- "Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles," by R. Eisberg and R. Resnick, John Wiley and Sons.
- "Atkins' Physical Chemistry," by P. Atkins and J. de Paula, W. H. Freeman and Company.
- "Electronic Properties of Crystalline Solids – An Introduction to Fundamentals," by R. H. Bube, Academic Press Inc.
- "Physical Chemistry: A Molecular Approach" by D. A. McQuarrie and J. D. Simon, University Science Books
- "Introduction to Solid State Physics" by C. Kittel, John Wiley and Sons
- "Solid State Physics", by N. W. Ashcroft and N. D. Mermin, Saunders College Publishing.
- MIT OpenCourseWare #5.61: "Physical Chemistry"
- "Elements of Quantum Mechanics" by Michael Fayer, (http://web.stanford.edu/group/fayer/book.html)

HOMEWORK:

- Homework will be assigned with due dates and will be posted to Canvas. The HW will be graded on a rough scale where:

  Very good (A): 85-100
  Good start but a few fundamental errors (B): 70-85
  Fundamental errors on multiple problems (C): 55-70
  Attempted, but did not know how to get started on multiple problems (D): 40-55
  Little meaningful progress (F): <40

- All homework solutions must be scanned to .pdf (be sure the scan is high quality) and submitted via Canvas (NOT VIA EMAIL).
- No late homework will be accepted.
- Solutions to the homework will be reviewed in class.

EXAMINATIONS:

There will be one mid-term and one final. The final is not comprehensive. The exams are closed book and closed notes except for (2) 8.5 in. X 11 in. sheets. Calculators may be required for certain problems. Calculators should not have information stored on them.

GRADES:

- The overall course grade will be determined based on the following: Homework (30%), Mid-term (35%), Final (35%)
- The following is the grading scale:

  A: 85-100
  B: 70-85
  C: 55-70
  D: 40-55
  F: <40

COURSE TIMELINE:

Lecture #	**Lecture Topic**	**Assignment**
1	Introduction, Examples, Origins of QM	
2	Schroedinger's equation and postulates	
3	Applications to simple systems	
4	Applications to simple systems	
5	Applications to simple systems	
6	Applications to atoms	
7	Applications to atoms	HW #1 (QM postulates and simple systems) is due
8	Review HW#1	
9	Applications to molecules	
10	Applications to molecules	HW #2 (application of QM to atoms) is due
11	Review HW#2 - Applications to molecules	
12	Free electron theory	
13	Free electron theory	HW #3 (application of QM to molecules) is due
14	Review HW#3/Exam 1	
15	MID-TERM EXAM	MID-TERM EXAM (postulates, simple systems, atoms, molecules)
16	Bloch and K-P	
17	3D energy bands	
18	3D energy bands	
19	Energy bands of real crystals	
20	Density of states	HW#4 (free electron theory and energy bands) is due
21	Carrier Statistics	
22	Dopants and Imperfections	
23	Dopants and Imperfections	
24	Excess Carriers	HW#5 is due (real energy bands, density of states, statistics, dopants)
25	Excess Carriers	
26	Transport&Scattering	
27	Transport&Scattering	
28	Transport&Scattering	
29	Review HW#6/Final Exam	HW#6 is due (excess carriers, transport, scattering)
	FINAL EXAM	FINAL EXAM

***RECOMMENDED BACKGROUND BY TOPIC:**

1. Crystal structure.
2. Fundamental laws and theories of classical physics and chemistry. Quantum mechanics will be covered as part of this course.
    - These topics represent recommended background for this course. Students should content the instructor with detailed questions regarding recommended background.

COVID

This class will be delivered in person. Accommodations will be made for any student that must quarantine.

Georgia Tech is committed to promoting a campus community that supports holistic well-being, as well as empowering students to make choices that enable positive health outcomes. As we continue to live and learn through a pandemic, Georgia Tech strongly encourages students to utilize several tools not only to reduce their own risks of infection from Covid-19, but also to help reduce the overall levels of transmission in the community.

These tools include:

1. Getting fully vaccinated. Getting vaccinated at Tech is easy and free.
2. Wearing face coverings consistently in all indoor settings and also in outdoor settings when in close proximity to others.
3. Getting tested on a regular basis, regardless of whether you are vaccinated or asymptomatic. No appointment is needed for Georgia Tech's asymptomatic testing, and it is free.
4. Avoiding touching your face until you have cleaned your hands with soap and water or used hand sanitizer.
5. Immediately self-quarantining or self-isolating if you experience any symptoms that could be related to Covid-19 or if you have tested positive for Covid-19.

Academic Integrity

Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. For information on Georgia Tech's Academic Honor Code, please visit http://www.catalog.gatech.edu/policies/honor-code/ or http://www.catalog.gatech.edu/rules/18/.
Any student suspected of cheating or plagiarizing on a quiz, exam, or assignment will be reported to the Office of Student Integrity, who will investigate the incident and identify the appropriate penalty for violations.

Accommodations for Students with Disabilities

If you are a student with learning needs that require special accommodation, contact the Office of Disability Services at (404)894-2563 or http://disabilityservices.gatech.edu/, as soon as possible, to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also e-mail me as soon as possible in order to set up a time to discuss your learning needs.

Attendance and/or Participation

Attendance is not mandatory, but students are responsible for all material presented and any announcements made during lectures.

Collaboration & Group Work

I encourage you to discuss and work together on your homework. However, you must submit your own answers and the answers should not be replicas. If it is apparent that the homework of several students are exact replicas, all students will receive a zero on that assignment.

Extensions, Late Assignments, & Re-Scheduled/Missed Exams

If a student has a legitimate conflict (e.g. athletic event, interview, religious observance) and will miss an exam, you **must reschedule the exam with me <u>at least</u> one week prior to the examination day**.

Student-Faculty Expectations Agreement

At Georgia Tech we believe that it is important to strive for an atmosphere of mutual respect, acknowledgement, and responsibility between faculty members and the student body. See http://www.catalog.gatech.edu/rules/22/ for an articulation of some basic expectation that you can have of me and that I have of you. In the end, simple respect for knowledge, hard work, and cordial interactions will help build the environment we seek. Therefore, I encourage you to remain committed to the ideals of Georgia Tech while in this class.