Chem 166 Quantum materials, where physics and chemistry meet

Meeting Times

Lecture: Every Mondays and Wednesdays, 12:00-1:15 pm Eastern Time

Section: Fridays, 12:00-1:15 pm Eastern Time

Students are highly encouraged to enroll for the timed section. If you are unable to attend any of the timed sections, or if they are at capacity, please enroll in the placeholder (TBA) section. In that case, you will be contacted after November 15. Pending approval from the Office of Undergraduate Education, we might be able to move you into a currently-offered section, or, in some circumstances, a new section time might be scheduled. Unfortunately, if neither of those options are possible, you will not be able to take the course.

Course Description

The discoveries of new materials have been so definitive that they are used to name periods in the history of mankind, such as Stone Age, Bronze Age, Iron Age, and Silicon Age. As we enter the quantum era, research focuses on *Quantum Materials*, where quantum mechanical effects are pronounced, holding promising for quantum computer, space technology, and clean energy. In this class, we will teach you the quantum theory of crystalline materials, including the cutting-edge quantum materials such as superconductors, magnets, topological insulators, light-harvesting materials, etc. We will teach these from a chemistry perspective, i.e., by drawing orbitals, chemical bonds and electron clouds in real space, in contrast to the typical quantum theory of solids in physics (solving Hamiltonians in momentum space). For chemistry and engineering students, we hope this class can teach you solid state theory without being bogged down by heavy math. For physics student, we hope this class can help you to establish a real space intuition for many of the concepts, which are lacking in present education. Overall, we hope to teach you the research frontiers in quantum science entered on materials discovery.

Instructor:
Prof. Su-Yang Xu
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Office Hours: TBD or by appointment

Teaching fellow
Mr. Ted Yu-fei Liu

Course Grading

- Group project during semester (presentation+paper) to discuss a frontier research paper 50%. Presentations will be held on the sections.
- Final project – use DFT to calculate the band structure of a material 40%
- Participation - 10%

Course Schedule (Tentative)

Part-I Foundation of the quantum theory of materials

1. Course introduction
2. Recap of H atom
3. Recap of H2+ molecule
4. Building bands from atoms #1, 1D H-chain
5. Building bands from atoms #2, graphene
6. Drude theory of conductivity
7. Band theory

Part-II Topological Insulators

8. Basic concepts
9. Graphene and Berry curvature
10. Band representation in 1D
11. Band representation in 2D

Part-III Magnetism

12. Isolated Magnetic Moments and Paramagnetism
13. Magnetic torque, magnetic force
14. Pauli exclusion and perturbation theory
15. Helium, perturbation theory
16. Exchange interaction, SOC
17. Ferromagnetism
18. Antiferromagnetism

Part-IV Superconductivity

19. History of superconductivity
20. Cooper pairing
21. Meissner effect

Part-V Light harvesting materials

22. Optical properties of materials
23. Intrinsic photocurrent
24. Review