MSE 674 Quantum and Energy Materials Fall 2023, W 2:15 – 4:30, Ferris 501

Instructor: Prof. T. Egami (208 South College, SWC B101C ORNL, egami@utk.edu)

This course is designed for graduate students in materials science, condensed matter physics, chemistry, nuclear engineering, chemical engineering and energy science and engineering, who are interested in learning physics of real materials related to quantum and energy applications. Because advanced materials used or researched today are more complex than traditional materials, simple concepts taught in introductory condensed matter physics courses are no longer sufficient in understanding their functionality. Focusing on how electrons behave in solids, various microscopic mechanisms to produce physical properties are introduced in this course. Also advanced experimental methods to study the electronic and atomic structures are discussed. Students will go through several extended exercises designed to understand the course materials in depth. Basic knowledge of quantum-mechanics and materials physics or condensed matter physics is required.

Textbook: *Atomic and Electronic Structure of Solids,* E. Kaxiras (Cambridge University Press, Cambridge, 2003): **Additional reading:** *Quantum Theory of Materials*, E. Kaxiras and J. D. Joannopoulos (Cambridge University Press, Cambridge, 2019), *Electronic Structure: Basic Theory and Practical Methods*. R. M. Martin (Cambridge University Press, Cambridge, 2004)

Time and Location: Wednesday 2:15 – 4:30 pm, Ferris 501.

Outline:

1. What is quantum mechanics?
   Idea of quantization, wave function, observables, Schrödinger equation, uncertainty, commutation relation.
2. Quantum and energy materials
   Quantum computing, nano-science, advanced energy materials, including solar-cells, superconductors, spintronics, and water, basis of quantum mechanics
3. Simple picture of electronic states in solids
   - 3-1. Free electron model
   - 3-2. Scattering by a periodic potential
   - 3-3. Band structure, Brillouin zone, Fermi level
   - 3-4. Bond and band
   - 3-5. Experimental detection: optical absorption, ARPES, x-ray diffraction
4. Electronic structure of real solids
   - 4-1. Hydrogen and other atoms
   - 4-2 The concept of pseudo-potential
   - 4-3. Periodic table
   - 4-4. Exchange and correlation, density functional theory
   - 4-5 Hubbard model
   - 4-6. Tight-binding model
   - 4-7. sp^3 bonds in Si and Ge
5. Metal, insulator and semiconductor

   - 5-1. Optical gap in semiconductor and insulator
   - 5-2. Plasma oscillation and optical response of a metal
   - 5-3. Response function of a metal, Friedel oscillation and Fermi surface nesting
   - 5-4. p-n junction, LED and solar cell
   - 5-5. Thermoelectric effect
6. Complex materials with disorder
   - 6-1. Concept of percolation
   - 6-2. Disorder and localized states
   - 6-3. Mobility edge
   - 6-4. Electronic states in alloys; split bands
   - 6-5. Coherent potential approximation
   - 6-6. Electronic states in liquids and glasses: Recursion method
7. Phonons and thermal effects
   - 7-1. Phonons, second quantization
   - 7-2. Phonon-phonon interaction
   - 7-3. Thermal conductivity
8. Superconductivity
   - 8-1. Superconductivity
   - 8-2. Frölich Hamiltonian
   - 8-3. BCS theory
   - 8-4. Cuprate high-temperature superconductors
   - 8-5. Josephson junction and quantum computing
9. Topological materials
   - 9-1. Spin-orbit coupling
   - 9-2. Band splitting
   - 9-3. Topology of the band structure
   - 9-4. Surface states
   - 9-5. Properties of topological materials
10. Spintronics
    - 10-1. Exchange interaction
    - 10-2. Stoner magnet, Stoner excitation
    - 10-3. Strong and weak magnetism, half-metallic state
    - 10-4. Magnetism of transition metals and Friedel model
    - 10-5. Spin Hall effect
    - 10-6. Spintronics

Grading will be based on homeworks, class discussion and two papers. The subject of the papers will be determined by proposal and discussion with the instructor.

Projects:

1. Band structure calculation
2. Recursion technique for random systems
3. Electronic susceptibility
4. Spin and magnetism